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Near Hartree-Fock Quality Gaussian Type Orbital Basis Sets for the First- and Third-Row Atoms

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SUMMARY

Energy–optimized, near Hartree–Fock quality Gaussian type orbital (GTO) basis sets are reported for the first–row (Li to Ne) and third–row (K to Kr) atoms. The most accurate basis sets reported for the first row are ($18\,s\;13\,p$) sets which are within 4 μE_H of the numerical Hartree–Fock (NHF) results. For B to Ne basis sets with more than $15s$ functions are quadruple zeta in the valence space. For the first–row transition metal atoms the ($20\,s\;12\,p\;9\,d$) basis sets are triple zeta in the valence space and are approximately equivalent to Clementi and Roetti's accurate Slater type orbital (STO) sets. Supplementing the ($20\,s\;12\,p\;9\,d$) basis sets optimized for the lowest state with the $4\,s^2\,3\,d^n$ occupation with a diffuse d function gives Self-Consistent-Field (SCF) energy separations to the $4\,s^1\,3\,d^{n+1}$ and $3\,d^{n+2}$ states which are within 100 μE_H of the NHF results. The most accurate basis sets for the transition metal atoms are within 30 μE_H of the NHF results. In addition, energy optimized sets are reported for He(^3P), Li(^2P) and Be(^3P).

INTRODUCTION

Recent studies (refs. 1–4) have demonstrated that for many calculations the major factor limiting the accuracy of electronic structure calculations are deficiencies in the one–particle basis sets. Almlöf and Taylor (ref. 5) have developed procedures for contracting large one–particle basis sets such that there is little contraction loss at either the self-consistent-field (SCF) or correlated level. In addition, vectorized integral codes (ref. 6) are available which can efficiently handle general contractions making it feasible to employ such basis sets in molecular calculations. Previous work on basis set selection has been the subject of recent reviews (refs.7–10) and two extensive compilations of basis sets have appeared (refs. 11–12). In this work, energy–optimized, near Hartree–Fock (HF) quality gaussian type orbital (GTO) basis sets are reported for the first– (Li–Ne) and third–row (K–Kr) atoms. The objective is to provide a selection of high quality, energy–optimized basis sets that are approximately energy balanced (energy balance implies that approximately the same energy lowering is obtained upon adding a single function of any symmetry and reoptimizing) and are at least triple zeta (TZ) in the valence space. For all of the systems reported in this work, when the valence space is TZ there are at least 3 GTO functions representing each SCF orbital. In addition, p polarization sets are reported for Li, He and Be. This work has been summarized in reference 13 and the basis sets are available from the Quantum Chemistry Program Exchange (QCPE, Bloomington, Indiana 47401).

METHODS

The orbital exponents were optimized by minimizing the restricted HF energy using a scaled Newton–Raphson scheme in which the Hessian is evaluated numerically using analytically determined gradients (ref. 15,16). The basis sets were optimized until the energy was stationary to at least 1×10^{-8} E_H and the virial ratio differed from 2 by less than 1×10^{-8}. While a virial ratio of 2 is not a sufficient condition for a minimum, it is a sensitive measure of convergence in the exponent optimization procedure. The energy usually stabilized well before the virial ratio. The basis sets reported are believed to correspond to "near" minimum solutions. However, numerical precision problems in accurately determining the Hessian made the absence (or presence) of negative eigenvalues an unreliable measure of convergence to a minimum. In part this occurs since there is a near linear dependency in the parameter space that results in a number of very small eigenvalues (ref. 14). The tight s and p functions for all of the basis sets reported obey the ratio relations reported in reference 14. No such relation is observed for the ratio of the d exponents.

The starting orbital exponents were selected in the following order of preference. First, derived sets where the exponents are taken from other optimized sets for the same atom and state. For example a $(24\,s\ 15\,p)$ set for K can be derived from the $(24\,s\ 12\,p)$ and $(23\,s\ 15\,p)$ sets. The energy improvement upon further optimization is minimal. Second, by scaling optimized sets for other atoms with similar spatial extent by the ratio of Z^2, where Z is the nuclear charge. The scaling works well for Be to Ne, Ga to Kr and for the first–row transition metal atoms having the same s occupation. The improvement upon optimization is generally small, especially when an adjacent atoms basis set is scaled. Third, by adding one function to each symmetry where the inner functions are specified by ratios given in reference 14. (For optimized basis sets the ratios between the tightest s and the tightest p functions are nearly independent of Z and the size of the basis set). This procedure worked well except when the number of functions describing the valence shell increases, say from double zeta (DZ) to TZ, and there is a sizable gap between the valence and outer–core exponents. Fourth, scaled basis sets that are extended with even–tempered functions. For example, an acceptable initial set of exponents for the s space may be obtained by scaling an appropriately sized H atom basis set. Note that simple even–tempered sets make a poor set of starting orbitals, particularly for large basis sets, because the even–tempered sets over specify the compact regions and the optimization procedure must significantly shift the exponents.

The numerical Hartree–Fock (NHF) energies were evaluated using a slightly modified version of the Cowan and Griffin code (ref. 17).

FIRST–ROW ATOMS

The most accurate energy–optimized GTO basis sets for the first–row atoms were the $(13\,s\ 8\,p)$ sets of van Duijneveldt (ref. 18), which are TZ in the valence space. (The $2\,s$ SCF orbital is TZ in that three GTO functions describe this orbital. It should be noted, however, that in this basis at the

correlated level four functions are required to recover most of the $2s$ correlation energy (ref. 5)). The average error in the SCF energies for the atoms B to Ne is 225 μE_H with the maximum error being 524 μE_H for Ne as compared to an average error of 20 μE_H for the HF–quality, Slater–type orbital basis sets given by Clementi and Roetti (ref. 19). For most applications these basis sets have been shown to provide an excellent description of both the atomic and molecular systems. Schmidt and Ruedenberg (ref.20) have reported formulas for generating even–tempered basis sets of arbitrary size which yield energies converging to the NHF results. Energy–optimized sets are slightly smaller than the corresponding even–tempered sets so there is some advantage in employing such sets. These basis sets have been employed in demonstrating basis set saturation for the nitrogen hyperfine coupling constant (ref. 21) and the dissociation energy of oxygen (ref. 22).

The HF atomic energies for the ground states of the first row atoms are reported in Table I for all of the basis sets generated and are compared with the NHF result. The $(13s\ 8p)$ sets derived in this work have an average error in the SCF energies for the atoms B to Ne of 191 μE_H with the maximum error being 421 μE_H for Ne. The errors are slightly smaller than for the sets reported by van Duijneveldt (ref. 18) and the basis sets are slightly more compact. For B to Ne the basis sets with more than $15s$ functions are quadruple zeta (QZ) in the valence region. Also reported in Table I are basis sets for He(^3P), Li(^2P), and Be(^3P). These basis sets should be useful for defining polarization sets for the atoms. Supplementary diffuse functions for describing the negative ions (Li to F) and their NHF energies are given in Table II.

THIRD–ROW ATOMS

The energies for the third row atoms are summarized in Table III and IV. Except for K, all the basis sets with 20 or more s functions are TZ in the valence space and none of the transition metal basis sets with 19 s orbitals are TZ. For K, 24 s functions are required for a TZ solution. As reported by Faegri (ref. 23), the transition metal basis set requirements for a constant error in the energy vary noticeably across the row. For representative systems the approximate energy lowering with the addition of each function is given in Table V and the energy balanced basis sets are given in Table VI. The SCF energies for all of the basis sets are reported in Table III and are compared with the NHF energies and the SCF energies of the accurate sets of Clementi and Roetti. The $(20s\ 12p\ 9d)$ sets are roughly equivalent in error compared to the NHF energy as are Clementi and Roetti's accurate sets. The most accurate basis sets reported are within 30 μE_H of the NHF energies. These basis sets have already been employed in a number of studies (refs. 24–27) which have shown their utility in quantitative investigations of transition–metal chemistry and spectroscopy.

To employ the basis sets optimized for the $4s^2 3d^n$ states to describe the other low lying atomic states or in molecular calculations it is necessary to supplement the basis sets with a diffuse $3d$ function. Optimized supplementary $3d$ functions for the $20s\ 12p\ 9d$ sets are reported in Table VII, along with the calculated SCF and NHF energies for the $4s^1 3d^{n+1}$ and $3d^{n+2}$ states. The energy separations are within 100 μE_H of the corresponding NHF result for all of the transition–metal atoms. This procedure results in a more balanced description of the states than starting with the

$4s^1 3d^{n+1}$ basis sets. Also note that p functions are required to describe the $4p$ orbital in molecular calculations. If these functions are optimized for the $3d^n 4s^1 4p^1$ occuptation then they are too diffuse for molecular calculations and must be scaled. (e.g. for Sc (^4F) the optimized supplementary functions for the ($20s\ 12p\ 9d$) set are 0.0769, 0.0286, and 0.01173 compared with the even–tempered exponents of 0.0911, 0.0376, and 0.01551). However, supplementing the present basis sets with three even–tempered p functions has proven to be quite adequate and, therefore, supplementary p functions have not been optimized. Supplementary $3d$ functions for the other basis sets are given in Table VIII.

For Ga to Kr the basis set sizes were selected by extending the energy balanced ($20s\ 12p\ 9d$) and ($21s\ 13p\ 10d$) transition metal sets with three p functions to describe the $4p$ orbital yielding basis sets of ($20s\ 15p\ 9d$) and ($21s\ 16p\ 10d$). The average error in the SCF energies compared with NHF are 738 and 289 μE_H respectively. This may be compared to the ($20s\ 14p\ 9d$) well–tempered sets of Huzinaga and Klobukowski (ref. 28) which have an average error of 4400 μE_H. There is thus a considerable energy improvement with exponent optimization. Supplementary diffuse functions and NHF energies for the negative ions (Ga to Br) are given in Table IX.

The basis set, the orbital exponents and eigenvectors for all of the basis sets optimized for this work are given in Tables X-CCXI.

CONCLUSIONS

High quality, energy–optimized, near Hartree–Fock quality GTO basis sets are reported for the first–row (Li to Ne) and the third–row (K to Kr) atoms. The most accurate sets are within 4 μE_H of the NHF energies for the first–row and within 30 μE_H for the transition metal atoms.

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Table I. Summary of atomic energies, E_H, for first–row atoms.

	Li(^2S)	Be(^1S)
13s	−7.432716	−14.573000
14s	−.432723	−.573012
15s	−.432725	−.573017
16s	−.4327261	−.5730208
17s	−.4327264	−.5730221
18s	−.4327266	−.5730227
NHF	−.432727	−.573023

	He(^3P)	Li(^2P)		Be(^3P)
10s 3p	−2.130650	−7.364248	13s 3p	−14.508941
10s 4p	−.131272	−.364866	13s 4p	−.510914
10s 5p	−.131398	−.365009	13s 5p	−.511351
10s 6p	−.131424	−.365042	13s 6p	−.511451
10s 7p	−.131430	−.3650505	13s 7p	−.511475
10s 8p	−.1314319	−.3650525	13s 8p	−.5114806
10s 9p	−.1314323	−.3650530	13s 9p	−.5114822
11s 9p	−.1314350	−.3650628	14s 9p	−.5114933
12s 9p		−.3650667	15s 9p	−.5114974
13s 9p		−.3650682	16s 9p	−.5114992
14s 10p		−.3650690	17s 10p	−.5115008
NHF	−.131437	−.365070		−.511502

	B(^2P)	C(^3P)	N(^4S)	O(^3P)	F(^2P)	Ne(^1S)
13s 8p	−24.529017	−37.688542	−54.400811	−74.809202	−99.409055	−128.546677
14s 9p	−.529040	−.688585	−.400883	−.809322	−.409239	−.546946
15s 10p	−.529052	−.688605	−.400914	−.809369	−.409308	−.547042
16s 11p	−.529057	−.688613	−.400926	−.809387	−.409333	−.547076
17s 12p	−.529059	−.688616	−.400931	−.809393	−.409342	−.547089
18s 13p	−.529060	−.688618	−.400933	−.809396	−.409346	−.547094
NHF	−.529061	−.688619	−.400934	−.809398	−.409349	−.547098

Table II. Supplementary functions for Li to F.

	Basis[a]	suplemental functions		Energy	NHF
		α_s	α_p		
$Li^-(^2S)$	Li(13*s*)	0.006119		-7.428208	-7.428232
	Li(14*s*)	0.006069		-7.428215	
	Li(15*s*)	0.006068		-7.428219	
$B^-(^3P)$	B(13*s* 8*p*)		0.015561	-24.518740	-24.519221
	B(13*s* 8*p*)	0.026903	0.015723	-24.519163	
	B(14*s* 9*p*)	0.026326	0.014644	-24.519190	
	B(15*s* 10*p*)	0.024054	0.013643	-24.519203	
	B(16*s* 11*p*)	0.023146	0.012841	-24.519211	
	B(17*s* 12*p*)	0.022397	0.012163	-24.519215	
	B(18*s* 13*p*)	0.021743	0.011544	-24.519217	
$C^-(^4S)$	C(13*s* 8*p*)	0.040893	0.027188	-37.708775	-37.708844
	C(14*s* 9*p*)	0.039541	0.025306	-37.708813	
	C(15*s* 10*p*)	0.036847	0.023857	-37.708829	
	C(16*s* 11*p*)	0.035322	0.022525	-37.708841	
	C(17*s* 12*p*)	0.034711	0.021199	-37.708841	
	C(18*s* 13*p*)	0.033728	0.020323	-37.708842	
$N^-(^3P)$	N(13*s* 8*p*)	0.053842	0.036844	-54.321846	-54.321959
	N(14*s* 9*p*)	0.051679	0.034307	-54.321909	
	N(15*s* 10*p*)	0.048441	0.032035	-54.321937	
	N(16*s* 11*p*)	0.044804	0.030533	-54.321950	
	N(17*s* 12*p*)	0.045511	0.028670	-54.321955	
	N(18*s* 13*p*)	0.047366	0.027275	-54.321957	
$O^-(^2P)$	*O*(13*s* 8*p*)	0.068424	0.044765	-74.789558	-74.789746
	O(14*s* 9*p*)	0.064934	0.041444	-74.789676	
	O(15*s* 10*p*)	0.061859	0.038822	-74.789718	
	O(16*s* 11*p*)	0.059761	0.036797	-74.789734	
	O(17*s* 12*p*)	0.057836	0.034655	-74.789741	
	O(18*s* 13*p*)	0.055937	0.032819	-74.789743	
$F^-(^1S)$	F(13*s* 8*p*)	0.084204	0.054884	-99.459202	-99.459454
	F(14*s* 9*p*)	0.080072	0.050993	-99.459356	
	F(15*s* 10*p*)	0.076143	0.047765	-99.459416	
	F(16*s* 11*p*)	0.072149	0.044881	-99.459439	
	F(17*s* 12*p*)	0.071507	0.042595	-99.459447	
	F(18*s* 13*p*)	0.069354	0.040714	-99.459451	

[a]The basis specifies the parent basis set to which the supplementary functions are

added. The energy is evaluated using the parent basis set plus the supplementary functions.

Table III. Summary of atomic energies, E_H, for third–row atoms.

	NHF	STO[a]	GTO		$\Delta(\mu E_h)$[b]
			Basis[c]	Energy	
K(^2S)	−599.164787	−.16453	20,12	−.164579	208
$4s^1$			24,12	−.164627	160
			21,13	−.164704	83
			22,14	−.164751	36
			23,15	−.164771	16
			24,15	−.164772	15
			25,16	−.164780	7
Ca(^1S)	−676.758185	−.75803	20,12	−.757915	270
$4s^2$			21,13	−.758079	106
			22,14	−.758140	45
			23,15	−.758166	19
			23,16	−.758166	19
Sc(^2D)	−759.735718	−.73552	20,12,9	−.735416	302
$4s^2 3d^1$			21,13,8	−.735562	156
			21,14,8	−.735580	138
			21,14,9	−.735629	89
			22,14,9	−.735658	60
			23,15,10	−.735693	25
			23,15,11	−.735695	23
Ti(^3F)	−848.405997	−.40575	20,12,9	−.405659	338
$4s^2 3d^2$			21,13,8	−.405786	211
			22,14,9	−.405920	77
			23,15,10	−.405967	30
			23,15,11	−.405971	26
V(^4F)	−942.884338	−.88420	20,12,8	−.883854	484
$4s^2 3d^3$			20,12,9	−.883959	379
			21,13,9	−.884163	175
			22,14,10	−.884269	69
			22,15,10	−.884287	51
			23,15,11	−.884309	29
Cr(^7S)	−1043.356377	−.3552	20,12,9	−.355952	425
$4s^1 3d^5$			22,14,10	−.356280	97
			23,15,11	−.356338	39
Cr(^5D)	−1043.309818	−.3095	20,12,9	−.309392	426
$4s^2 3d^4$			21,13,10	−.309655	163
			22,14,10	−.309739	79

			22,15,11	−.309769	49
			23,15,11	−.309785	33
			24,16,12	−.309804	14
Mn(^6S)	−1149.866252	−.8657	20,12,9	−.865774	478
$4s^2 3d^5$			21,13,10	−.866071	181
			22,14,10	−.866161	91
			23,15,11	−.866215	37
			24,16,12	−.866235	17
Fe(^5D)	−1262.443664	−.4432	20,12,9	−.443122	542
$4s^2 3d^6$			21,13,10	−.443462	202
			22,14,10	−.443559	105
			23,15,11	−.443623	41
			24,16,12	−.443647	17
Co(^4F)	−1381.414551	−.4142	19,12,8	−.413447	1104
$4s^2 3d^7$			20,12,8	−.413522	1029
			20,12,9	−.413937	614
			21,13,10	−.414325	226
			22,14,10	−.414429	122
			22,15,11	−.414484	67
			23,15,11	−.414504	47
			24,16,12	−.414532	19
Ni(^3F)	−1506.870907	−.8705	19,13,8	−.869768	1139
$4s^2 3d^8$			20,13,8	−.869853	1054
			20,12,9	−.870211	696
			20,13,9	−.870391	516
			21,13,10	−.870653	254
			22,14,10	−.870765	142
			22,15,11	−.870831	76
			23,15,11	−.870853	54
			23,16,12	−.870874	33
			24,16,12	−.870885	22
Ni(^3D)	−1506.824027	−.8224	20,12,9	−.823185	823
$4s^1 3d^9$			21,13,10	−.823725	302
			22,14,10	−.823842	185
			23,15,11	−.823959	68
			24,16,12	−.823990	37
Cu(^2S)	−1638.963741	−.9628	20,12,9	−.962880	861
$4s^1 3d^{10}$			22,14,10	−.963529	212
			23,15,11	−.963664	77
Cu(^2D)	−1638.950080	−.9496	20,12,9	−.949295	785
$4s^2 3d^9$			21,13,10	−.949796	284

			21,14,10	−.949864	216
			22,14,10	−.949916	164
			23,15,11	−.950018	62
			24,16,12	−.950055	25
$Zn(^1S)$	−1777.848115	−.8477	20,12,9	−.8472335	882
$4s^2 3d^{10}$			21,13,10	−.847799	316
			22,14,10	−.847927	188
			23,15,11	−.848045	70
			24,16,12	−.848087	28

[a]Clementi and Roetti, Ref. 19.
[b]Difference between GTO and NHF energies in μE_h.
[c]The number of s, p, and d primitives.

Table IV. Summary of atomic energies, E_H, for Ga to Kr.

	$20s\ 15p\ 9d$	$21s\ 16p\ 10d$	NHF
Ga(^2P)	−1923.260286	−.260738	−.261010
Ge(^3P)	−2075.359023	−.359458	−.359734
As(^4S)	−2234.237946	−.238373	−.238654
Se(^3P)	−2399.866873	−.867316	−.867611
Br(^2P)	−2572.440569	−.441030	−.441333
Kr(^1S)	−2752.054193	−.054669	−.054976

Table V. Approximate energy lowering, μE_h, obtained by adding an additional function

	Sc	Ti	V	Co	Ni
19–20s	120	94		75	85
20–21s	79	79	82	106	114
21–22s	48	35	39	46	49
22–23s	13	19	15	20	20
12–13p	134	131	111	167	179
13–14p	49	47	48	59	64
14–15p	14	13	17	23	24
15–16p	6	9	8	11	13
8–9d	30	60	103	415	538
9–10d	8	17	29	114	148
10–11d			8	33	42
11–12d				9	12

Table VI. Approximately energy balanced basis sets

Sc, Ti	V	Co, Ni
$19s\ 12p\ 7d^a$	$20s\ 12p\ 8d$	$20s\ 12p\ 9d$
$21s\ 13p\ 8d$	$21s\ 13p\ 9d$	$21s\ 13p\ 10d$
$22s\ 14p\ 9d$	$22s\ 14p\ 10d$	$22s\ 14p\ 10d$
$23s\ 15p\ 10d$	$23s\ 15p\ 11d$	$24s\ 16p\ 12d$

[a] $4s$ space is DZ.

Table VII. Energies, E_H, of transition metal $4s^1 3d^{n+1}$ and $3d^{n+2}$ states and supplementary $3d$ functions for $(20s\ 12p\ 9d)$ basis sets.

$4s^1 3d^{n+1}$ states

state	supplementary $3d^a$	energy(E_H)	NHF
Sc(^4F)	0.027467	−759.698445	−.698786
Ti(^5F)	0.035094	−848.385779	−.386154
V(^6D)	0.040908	−942.879369	−.879783
Cr(^7S)	0.045794	−1043.355915	−.356377
Mn(^6D)	0.053051	−1149.743444	−.743958
Fe(^5F)	0.054670	−1262.377032	−.377616
Co(^4F)	0.058088	−1381.357723	−.358382
Ni(^3D)	0.060931	−1506.823281	−.824027
Cu(^2S)	0.065039	−1638.962898	−.963741

$3d^{n+2}$ states

state	energy(E_H)	NHF
Sc(^4F)	−759.571100	−.571455
Ti(^5D)	−848.249216	−.249621
V(^6S)	−942.763752	−.764209
Cr(^5D)	−1043.097800	−.098315
Mn(^4F)	−1149.529188	−.529826
Fe(^3F)	−1262.168821	−.169463
Co(^2D)	−1381.154812	−.155536
Ni(^1S)		−.669759

[a]The supplementary $3d$ function is optimized for the sd^{n+1} states. The energy is then determined in the resulting $(20s\ 12p\ 10d)$ basis set.

Table VIII. Supplementary d functions for the $4s^13d^{n+1}$ states of the first–row transition metal atoms.

	Basis[a]	suplemental function	Energy
Sc(^4F)	21s13p8d	0.03055	-759.698588
	21s14p9d	0.02746	-759.698672
	22s14p9d	0.02744	-759.698703
Ti(^5F)	21s13p8d	0.03931	-848.385909
	22s14p9d	0.03517	-848.386058
	23s15p10d	0.03208	-848.386111
	23s15p11d	0.02959	-848.386118
V(^6D)	20s12p8d	0.04597	-942.879260
	21s13p9d	0.04095	-942.879587
	22s14p10d	0.03710	-942.879701
	23s15p11d	0.03402	-942.879745
Cr(^7S)	21s13p10d	0.04126	-1043.356195
	22s14p10d	0.04125	-1043.356284
	23s15p11d	0.03763	-1043.356335
Mn(^6D)	21s13p10d	0.04794	-1149.743768
	22s14p10d	0.04796	-1149.743865
	23s15p11d	0.04380	-1149.743922
Fe(^5F)	21s13p10d	0.04924	-1262.377401
	22s14p10d	0.04921	-1262.377505
	23s15p11d	0.04836	-1262.377575
Co(^4F)	21s13p10d	0.05025	-1381.358128
	22s14p10d	0.05205	-1381.358240
	23s15p11d	0.04734	-1381.358320
	24s16p12d	0.04362	-1381.358351
Ni(^3D)	21s13p10d	0.05514	-1506.823739
	22s14p10d	0.05511	-1506.823861
	23s15p11d	0.05004	-1506.823953
	24s16p12d	0.04594	-1506.823990
Cu(^2S)	21s13p10d	0.05804	-1638.963416
	22s14p10d	0.05799	-1638.963653
	23s15p11d	0.05257	-1638.963653
	24s16p12d	0.04799	-1653.963695

[a]The basis specifies the parent basis set for the $4s^23d^n$ state to which the supplementary functions are added. The energy is evaluated using the parent basis set plus the supplementary functions.

Table IX. Supplementary functions for K, Ca and Ga to Br.

	Basis[a]	suplemental functions		Energy	NHF
		α_s	α_p		
$K^-(^2S)$	K(20s12p)	0.00497		-599.161616	-599.161916
	K(23s15p)	0.00482		-599.161880	
	K(24s15p)	0.00358		-599.161900	
	K(25s16p)	0.00363		-599.161909	
$Ga^-(^3P)$	Ga(20s15p9d)	0.01880	0.01182	-1923.259634	-1293.260381
	Ga(21s16p10d)	0.18963	0.1137	-1923.259634	
$Ge^-(^4S)$	Ge(20s15p9d)	0.02583	0.01857	-2075.393995	-2075.394742
	Ge(21s16p10d)	0.02605	0.01857	-2075.394485	
$As^-(^3P)$	As(20s15p9d)	0.03011	0.02458	-2234.222257	-2234.222939
	As(21s16p10d)	0.03251	0.02372	-2234.222681	
$Se^-(^2P)$	Se(20s15p9d)	0.03919	0.02828	-2399.904033	-2399.904726
	Se(21s16p10d)	0.03817	0.02660	-2399.904457	
$Br^-(^1S)$	Br(20s15p9d)	0.04547	0.03282	-2572.535562	-2572.536272
	Br(21s16p10d)	0.04389	0.03017	-2572.535999	

	Basis[a]	suplemental functions			Energy	NHF
		α_p	α_p	α_p		
$K(^2P)$	K(20s12p)	0.01214	0.02937	0.07873	-599.112899	-599.113144
	K(21s13p)	0.01019	0.02255	0.05176	-599.113067	
	K(22s14p)	0.01034	0.02271	0.05106	-599.113112	
	K(23s15p)	0.01002	0.02164	0.04763	-599.113131	
	K(25s16p)	0.01001	0.02183	0.04762	-599.113138	
$Ca(^3P)$	Ca(20s12p)	0.01997	0.04593	0.10419	-676.718513	-676.718768
	Ca(21s13p)	0.01864	0.01416	0.08847	-676.718672	
	Ca(22s14p)	0.01673	0.03545	0.07369	-676.718729	
	Ca(23s15p)	0.01497	0.03036	0.06110	-676.718753	

[a]The basis specifies the parent basis set to which the supplementary functions are added. The energy is evaluated using the parent basis set plus the supplementary functions.

Table X. He ^3P $(10s3p)$ basis set, orbital energies and eigenvectors. Energy(E_H) = -2.130650

	s space
Exponent	1s
	-1.734546
5409.967	0.000061
810.4816	0.000475
184.4496	0.002490
52.23195	0.010390
17.03032	0.036517
6.140957	0.108157
2.388893	0.254004
0.983297	0.400869
0.416422	0.295104
0.153862	0.040748
	p space
Exponent	2p
	-0.130769
0.585217	0.081973
0.111217	0.427020
0.030301	0.652556

Table XI. He ^3P $(10s4p)$ basis set, orbital energies and eigenvectors. Energy(E_H) $= -2.131272$

	s space
Exponent	1s
	−1.733865
5364.290	0.000062
803.6376	0.000480
182.8916	0.002515
51.79054	0.010498
16.88630	0.036882
6.088962	0.109142
2.368583	0.255707
0.974782	0.402082
0.411907	0.292502
0.150976	0.039013
	p space
Exponent	2p
	−0.131397
1.329799	0.028335
0.272794	0.155655
0.074826	0.503420
0.024562	0.490513

Table XII. He ^3P $(10s5p)$ basis set, orbital energies and eigenvectors. Energy(E_H) $= -2.131398$

	s space
Exponent	1s
	−1.733762
5363.510	0.000062
803.5209	0.000480
182.8650	0.002516
51.78302	0.010500
16.88385	0.036887
6.088112	0.109151
2.368048	0.255813
0.974579	0.401844
0.412174	0.292404
0.151302	0.039235
	p space
Exponent	2p
	−0.131523
2.638523	0.010292
0.595438	0.059840
0.166463	0.227989
0.055919	0.524961
0.020765	0.360913

Table XIII. He ^3P $(10s6p)$ basis set, orbital energies and eigenvectors. Energy(E_H) $= -2.131424$

	s space
Exponent	1s
	−1.733745
5369.213	0.000062
804.3748	0.000479
183.0593	0.002513
51.83806	0.010486
16.90180	0.036840
6.094541	0.109024
2.370804	0.255522
0.975695	0.401851
0.412495	0.292801
0.151394	0.039317
	p space
Exponent	2p
	−0.131550
4.936549	0.003749
1.164363	0.025032
0.345056	0.095443
0.116675	0.290392
0.044622	0.508321
0.018106	0.263405

Table XIV. He ^3P $(10s7p)$ basis set, orbital energies and eigenvectors. Energy(E_H) $= -2.131430$

	s space
Exponent	1s
	−1.733742
5364.525	0.000062
803.6729	0.000480
182.8996	0.002515
51.79284	0.010497
16.88708	0.036878
6.089198	0.109132
2.368538	0.255744
0.974772	0.401888
0.412160	0.292487
0.151240	0.039210
	p space
Exponent	2p
	−0.131556
8.914173	0.001385
2.124859	0.010516
0.667001	0.042483
0.230986	0.133813
0.088846	0.336898
0.037222	0.469837
0.016151	0.192362

Table XV. He ^3P $(10s8p)$ basis set, orbital energies and eigenvectors. Energy(E_H) $= -2.131432$

	s space
Exponent	1s
	−1.733741
5366.901	0.000062
804.0284	0.000480
182.9805	0.002514
51.81571	0.010491
16.89449	0.036859
6.091962	0.109074
2.369716	0.255630
0.975253	0.401862
0.412343	0.292650
0.151330	0.039272
	p space
Exponent	2p
	−0.131558
15.62045	0.000528
3.722562	0.004347
1.202176	0.019765
0.434827	0.062163
0.168838	0.172528
0.071261	0.366722
0.031987	0.420947
0.014640	0.140700

Table XVI. He ^3P $(10s9p)$ basis set, orbital energies and eigenvectors. Energy(E_H) $= -2.131432$

	s space
Exponent	1s
	−1.733741
5365.953	0.000062
803.8866	0.000480
182.9482	0.002515
51.80661	0.010494
16.89153	0.036867
6.090809	0.109099
2.369220	0.255678
0.975049	0.401874
0.412263	0.292582
0.151290	0.039245
	p space
Exponent	2p
	−0.131558
26.82582	0.000207
6.378491	0.001778
2.077046	0.009015
0.779104	0.030359
0.309902	0.083721
0.131282	0.208310
0.059394	0.381127
0.028136	0.369737
0.013446	0.103629

Table XVII. He ^3P $(11s9p)$ basis set, orbital energies and eigenvectors. Energy(E_H) $= -2.131435$

	s space
Exponent	1s
	-1.733743
9784.992	0.000029
1465.600	0.000227
333.5359	0.001190
94.45984	0.004996
30.80686	0.017861
11.11489	0.055365
4.329665	0.145408
1.790361	0.297486
0.773452	0.390583
0.337894	0.217528
0.112073	0.018376

	p space
Exponent	2p
	-0.131559
26.76149	0.000208
6.363414	0.001785
2.072282	0.009045
0.777394	0.030433
0.309335	0.083850
0.131119	0.208464
0.059341	0.381175
0.028118	0.369466
0.013440	0.103459

Table XVIII. Li ^2S $(13s)$ basis set. Energy$(E_H) = -7.432716$

	s space	
Exponent	1s	2s
	−2.477732	−0.196323
14773.87	0.000043	−0.000007
2213.137	0.000334	−0.000052
503.6660	0.001749	−0.000274
142.6378	0.007304	−0.001145
46.51530	0.025664	−0.004061
16.76436	0.075895	−0.012218
6.485126	0.181059	−0.030522
2.624750	0.325375	−0.060122
1.095155	0.373472	−0.095929
0.459970	0.167448	−0.112220
0.093919	0.006886	0.311921
0.044581	−0.003191	0.568907
0.020748	0.001135	0.226041

Table XIX. Li ^2S $(14s)$ basis set. Energy$(E_H) = -7.432723$

	s space	
Exponent	1s	2s
	−2.477738	−0.196323
29493.00	0.000018	−0.000003
4417.101	0.000141	−0.000022
1005.223	0.000739	−0.000115
284.7009	0.003107	−0.000487
92.86543	0.011135	−0.001746
33.51179	0.034670	−0.005520
13.04180	0.092171	−0.014928
5.357536	0.199576	−0.034207
2.279338	0.328836	−0.062156
0.993990	0.345975	−0.095904
0.433471	0.142761	−0.103973
0.095566	0.005319	0.307162
0.044657	−0.002101	0.579033
0.020633	0.000815	0.223215

Table XX. Li ^2S $(15s)$ basis set. Energy$(E_H) = -7.432725$

	s space	
Exponent	1s	2s
	−2.477740	−0.196323
57340.43	0.000008	−0.000001
8586.523	0.000061	−0.000010
1954.060	0.000322	−0.000051
553.4696	0.001360	−0.000212
180.5574	0.004917	−0.000773
65.17958	0.015709	−0.002466
25.41221	0.044354	−0.007108
10.51247	0.107763	−0.017568
4.537699	0.214768	−0.037436
2.014903	0.328001	−0.063539
0.913187	0.319501	−0.095462
0.411601	0.122928	−0.096403
0.096911	0.004280	0.302387
0.044877	−0.001440	0.585013
0.020636	0.000625	0.223983

Table XXI. Li ^2S $(16s)$ basis set. Energy$(E_H) = -7.432726$

	s space	
Exponent	1s	2s
	−2.477741	−0.196323
108401.4	0.000004	−0.000001
16230.85	0.000028	−0.000004
3693.639	0.000146	−0.000023
1046.225	0.000615	−0.000096
341.3346	0.002234	−0.000348
123.2364	0.007224	−0.001138
48.07162	0.021049	−0.003310
19.93437	0.054702	−0.008829
8.671334	0.122826	−0.020164
3.904202	0.227383	−0.040351
1.800662	0.323850	−0.064439
0.845141	0.293734	−0.094734
0.392653	0.106333	−0.089119
0.097806	0.003531	0.299849
0.045012	−0.001007	0.588524
0.020642	0.000504	0.224541

Table XXII. Li ^2S $(17s)$ basis set. Energy$(E_H) = -7.432726$

	s space	
Exponent	1s	2s
	−2.477741	−0.196323
197161.3	0.000002	0.000000
29516.17	0.000013	−0.000002
6716.082	0.000069	−0.000011
1902.227	0.000291	−0.000045
620.6299	0.001061	−0.000167
224.0993	0.003454	−0.000539
87.43531	0.010221	−0.001615
36.28587	0.027551	−0.004342
15.83308	0.066472	−0.010817
7.187959	0.138687	−0.022949
3.359890	0.238999	−0.043319
1.606216	0.316567	−0.065059
0.780626	0.266278	−0.093710
0.374195	0.090837	−0.081211
0.098292	0.002917	0.299659
0.045024	−0.000685	0.590467
0.020622	0.000415	0.224023

Table XXIII. Li ^2S ($18s$) basis set. Energy(E_H) = -7.432727

	s space	
Exponent	1s	2s
	−2.477741	−0.196323
305117.9	0.000001	0.000000
45621.81	0.000008	−0.000001
10368.83	0.000040	−0.000006
2933.582	0.000170	−0.000027
956.0815	0.000620	−0.000097
344.8592	0.002026	−0.000318
134.4151	0.006043	−0.000943
55.73306	0.016564	−0.002629
24.31260	0.041399	−0.006565
11.05835	0.091875	−0.015162
5.198821	0.174145	−0.029408
2.510701	0.267425	−0.050946
1.248470	0.300925	−0.068420
0.641101	0.202435	−0.091727
0.329759	0.057565	−0.059184
0.097957	0.001811	0.307071
0.044599	−0.000186	0.590373
0.020462	0.000279	0.218371

Table XXIV. Li ^2P $(10s3p)$ basis set, orbital energies and eigenvectors. Energy(E_H) $= -7.364248$

	s space
Exponent	1s
	−2.532161
11802.95	0.000057
1768.249	0.000442
402.4223	0.002314
113.9618	0.009627
37.15850	0.033490
13.38004	0.096615
5.158095	0.219780
2.074917	0.362559
0.859244	0.343387
0.353903	0.094748
	p space
Exponent	2p
	−0.127862
0.564113	0.073265
0.104659	0.426170
0.028919	0.655216

Table XXV. Li ^2P ($10s4p$) basis set, orbital energies and eigenvectors. Energy(E_H) $= -7.364866$

	s space
Exponent	1s
	−2.530995
11798.69	0.000057
1767.608	0.000442
402.2752	0.002314
113.9196	0.009631
37.14435	0.033504
13.37464	0.096653
5.155841	0.219846
2.073916	0.362576
0.858916	0.343287
0.353609	0.094738
	p space
Exponent	2p
	−0.128482
1.533878	0.022785
0.274931	0.139106
0.073622	0.500433
0.024027	0.508438

Table XXVI. Li ^2P $(10s5p)$ basis set, orbital energies and eigenvectors. Energy(E_H) $= -7.365009$

	s space	
Exponent	1s	2s
	−2.530776	
11793.71	0.000057	
1766.864	0.000442	
402.1057	0.002316	
113.8715	0.009636	
37.12868	0.033520	
13.36897	0.096695	
5.153618	0.219916	
2.072999	0.362657	
0.858392	0.343248	
0.353318	0.094570	

	p space
Exponent	2p
	−0.128626
3.266286	0.008630
0.651140	0.047526
0.169621	0.209780
0.055777	0.528552
0.020500	0.382716

Table XXVII. Li ^2P $(10s6p)$ basis set, orbital energies and eigenvectors. Energy$(E_H) = -7.365042$

	s space
Exponent	1s
	−2.530732
11792.05	0.000057
1766.614	0.000442
402.0490	0.002316
113.8555	0.009638
37.12345	0.033525
13.36708	0.096709
5.152846	0.219946
2.072679	0.362661
0.858318	0.343200
0.353303	0.094564
	p space
Exponent	2p
	−0.128659
6.249709	0.003388
1.369972	0.019314
0.367218	0.079091
0.119203	0.274108
0.044738	0.519502
0.017949	0.284408

Table XXVIII. Li ^2P $(10s7p)$ basis set, orbital energies and eigenvectors. Energy$(E_H) = -7.365050$

	s space
Exponent	1s
	−2.530723
11792.98	0.000057
1766.753	0.000442
402.0806	0.002316
113.8645	0.009637
37.12637	0.033522
13.36814	0.096700
5.153296	0.219928
2.072858	0.362658
0.858360	0.343227
0.353306	0.094571
	p space
Exponent	2p
	−0.128667
11.27960	0.001346
2.596328	0.008605
0.747648	0.032605
0.242443	0.116029
0.090648	0.325023
0.037362	0.486815
0.016036	0.210485

Table XXIX. Li ^2P $(10s8p)$ basis set, orbital energies and eigenvectors. Energy(E_H) $= -7.365052$

	s space
Exponent	1s
	−2.530721
11792.21	0.000057
1766.637	0.000442
402.0540	0.002316
113.8568	0.009637
37.12387	0.033525
13.36722	0.096708
5.152907	0.219942
2.072704	0.362663
0.858311	0.343208
0.353292	0.094560
	p space
Exponent	2p
	−0.128669
19.66353	0.000540
4.623111	0.003865
1.413783	0.015170
0.473721	0.049198
0.176151	0.154662
0.072675	0.360073
0.032141	0.441871
0.014556	0.156007

Table XXX. Li ^2P ($10s9p$) basis set, orbital energies and eigenvectors. Energy(E_H) $= -7.365053$

	s space
Exponent	1s
	−2.530720
11792.58	0.000057
1766.694	0.000442
402.0672	0.002316
113.8607	0.009637
37.12514	0.033524
13.36770	0.096704
5.153113	0.219935
2.072784	0.362660
0.858337	0.343218
0.353299	0.094566
	p space
Exponent	2p
	−0.128670
33.33459	0.000221
7.897605	0.001724
2.498380	0.007440
0.880599	0.023043
0.330599	0.069210
0.135926	0.192064
0.060377	0.380119
0.028235	0.392026
0.013364	0.115758

Table XXXI. Li ^2P $(11s9p)$ basis set, orbital energies and eigenvectors. Energy(E_H) $= -7.365063$

	s space
Exponent	1s
	−2.530724
22648.85	0.000025
3392.318	0.000196
772.0134	0.001028
218.6462	0.004311
71.31444	0.015356
25.72682	0.047071
9.996166	0.120859
4.087115	0.246138
1.726693	0.362998
0.746129	0.298311
0.316269	0.066872

	p space
Exponent	2p
	−0.128671
33.35775	0.000221
7.902985	0.001722
2.500165	0.007433
0.881303	0.023022
0.330851	0.069156
0.136002	0.191986
0.060402	0.380088
0.028243	0.392140
0.013367	0.115837

Table XXXII. Li ^2P $(12s9p)$ basis set, orbital energies and eigenvectors. Energy$(E_H) = -7.365067$

	s space
Exponent	1s
	−2.530725
41954.50	0.000012
6282.917	0.000091
1429.829	0.000476
404.9747	0.002006
132.1061	0.007230
47.68215	0.022870
18.57827	0.063067
7.665113	0.146160
3.287847	0.269349
1.447570	0.356026
0.647851	0.251835
0.279008	0.044114
	p space
Exponent	2p
	−0.128671
33.37342	0.000221
7.906711	0.001721
2.501374	0.007429
0.881731	0.023011
0.330977	0.069136
0.136034	0.191958
0.060412	0.380082
0.028246	0.392185
0.013368	0.115865

Table XXXIII. Li ^2P $(13s9p)$ basis set, orbital energies and eigenvectors. Energy(E_H) = -7.365068

	s space
Exponent	1s
	-2.530726
74718.71	0.000006
11188.30	0.000044
2546.139	0.000232
721.1808	0.000978
235.2752	0.003545
84.93513	0.011395
33.12063	0.032687
13.71652	0.082080
5.941083	0.173108
2.651974	0.289842
1.209217	0.341078
0.556503	0.202831
0.237586	0.025460

	p space
Exponent	2p
	-0.128672
33.37598	0.000221
7.907316	0.001721
2.501560	0.007428
0.881780	0.023011
0.330977	0.069141
0.136030	0.191964
0.060411	0.380083
0.028246	0.392178
0.013368	0.115860

Table XXXIV. Li ^2P $(14s10p)$ basis set, orbital energies and eigenvectors. Energy$(E_H) = -7.365069$

	s space
Exponent	1s
	−2.530726
126503.2	0.000003
18943.79	0.000023
4312.194	0.000120
1222.406	0.000506
399.2138	0.001837
144.2833	0.005945
56.33604	0.017396
23.38042	0.045748
10.18201	0.105149
4.592960	0.202320
2.121468	0.306685
0.996910	0.315394
0.468561	0.150648
0.187515	0.011547
	p space
Exponent	2p
	−0.128672
55.51916	0.000092
13.17503	0.000761
4.238383	0.003616
1.554368	0.011711
0.602069	0.032453
0.247580	0.091427
0.109730	0.225391
0.051617	0.386946
0.025250	0.342820
0.012398	0.086495

Table XXXV. Be ^1S $(13s)$ basis set. Energy$(E_H) = -14.573000$

	s space	
Exponent	1s	2s
	−4.732655	−0.309262
29156.37	0.000039	−0.000007
4367.459	0.000301	−0.000055
993.9501	0.001581	−0.000290
281.5011	0.006612	−0.001203
91.81760	0.023335	−0.004337
33.12042	0.069924	−0.013068
12.85704	0.170807	−0.034203
5.251469	0.317166	−0.068684
2.225906	0.376955	−0.118484
0.954220	0.184096	−0.106398
0.250765	0.009508	0.266056
0.102940	−0.003078	0.583896
0.041899	0.000807	0.279591

Table XXXVI. Be ^1S $(14s)$ basis set. Energy$(E_H) = -14.573012$

	s space	
Exponent	1s	2s
	−4.732662	−0.309264
54618.89	0.000018	−0.000003
8180.127	0.000138	−0.000025
1861.618	0.000723	−0.000131
527.2788	0.003039	−0.000558
172.0159	0.010905	−0.001988
62.10194	0.034047	−0.006372
24.20541	0.091201	−0.017219
9.992550	0.199278	−0.040861
4.304512	0.329340	−0.074235
1.921242	0.340423	−0.119205
0.866273	0.143811	−0.087821
0.247480	0.006487	0.278945
0.100870	−0.001847	0.583493
0.041287	0.000475	0.268870

Table XXXVII. Be ^1S $(15s)$ basis set. Energy$(E_H) = -14.573017$

	s space	
Exponent	1s	2s
	−4.732664	−0.309268
70103.33	0.000013	−0.000002
10498.76	0.000101	−0.000018
2389.295	0.000529	−0.000097
676.7329	0.002229	−0.000407
220.7551	0.008031	−0.001472
79.67718	0.025379	−0.004690
31.04373	0.069837	−0.013207
12.81153	0.161094	−0.031852
5.505751	0.292119	−0.063978
2.438160	0.362272	−0.104077
1.095148	0.214081	−0.120318
0.428756	0.024900	0.023953
0.199588	−0.003348	0.363870
0.085444	0.001009	0.539499
0.037132	−0.000243	0.196028

Table XXXVIII. Be ^1S $(16s)$ basis set. Energy$(E_H) = -14.573021$

	s space	
Exponent	1s	2s
	−4.732668	−0.309269
126512.3	0.000006	−0.000001
18942.46	0.000048	−0.000009
4310.405	0.000254	−0.000046
1220.803	0.001069	−0.000195
398.2395	0.003877	−0.000709
143.7553	0.012459	−0.002286
56.05460	0.035714	−0.006655
23.21624	0.089575	−0.017083
10.06369	0.188126	−0.038114
4.506501	0.309294	−0.070226
2.068805	0.338569	−0.108770
0.953986	0.167482	−0.105294
0.345883	0.013902	0.091499
0.167457	−0.003146	0.399744
0.075870	0.001019	0.489535
0.034438	−0.000243	0.151971

Table XXXIX. Be ^1S $(17s)$ basis set. Energy$(E_H) = -14.573022$

	s space	
Exponent	1s	2s
	−4.732669	−0.309269
231252.2	0.000003	−0.000001
34620.13	0.000023	−0.000004
7878.528	0.000119	−0.000022
2231.647	0.000504	−0.000092
728.0807	0.001833	−0.000334
262.8614	0.005944	−0.001090
102.5317	0.017443	−0.003208
42.52479	0.046076	−0.008647
18.52170	0.106765	−0.020569
8.372462	0.207263	−0.042859
3.890686	0.314064	−0.073978
1.848495	0.311840	−0.109056
0.878999	0.137868	−0.092791
0.327248	0.009829	0.120271
0.156130	−0.002098	0.415795
0.071987	0.000700	0.465951
0.033257	−0.000167	0.134034

Table XL. Be ^1S $(18s)$ basis set. Energy$(E_H) = -14.573023$

	s space	
Exponent	1s	2s
	−4.732669	−0.309269
408935.4	0.000001	0.000000
61225.01	0.000011	−0.000002
13932.70	0.000058	−0.000011
3946.398	0.000247	−0.000045
1287.506	0.000901	−0.000165
464.8390	0.002937	−0.000536
181.3289	0.008722	−0.001603
75.23308	0.023710	−0.004378
32.82357	0.058243	−0.011017
14.91237	0.125426	−0.024468
6.988313	0.225859	−0.047811
3.357053	0.314746	−0.077678
1.647082	0.281122	−0.108206
0.808129	0.110148	−0.078879
0.314569	0.006824	0.141653
0.148633	−0.001269	0.426499
0.069312	0.000421	0.448248
0.032418	−0.000099	0.121822

Table XLI. Be ^3P ($13s3p$) basis set, orbital energies and eigenvectors. Energy(E_H) $= -14.508941$

	s space
Exponent	1s
	−4.745294
29594.76	0.000038
4433.131	0.000296
1008.891	0.001551
285.7234	0.006490
93.18406	0.022929
33.60263	0.068838
13.03434	0.169007
5.314314	0.315813
2.243059	0.379185
0.954622	0.186521
0.250217	0.010820
0.112630	−0.003762
0.049747	0.000851
	p space
Exponent	2p
	−0.238910
1.484575	0.088809
0.288942	0.449212
0.075438	0.634367

Table XLII. Be ^3P ($13s4p$) basis set, orbital energies and eigenvectors. Energy(E_H) $= -14.510914$

	s space
Exponent	1s
	−4.743912
29974.35	0.000038
4489.970	0.000291
1021.826	0.001527
289.3879	0.006388
94.38012	0.022579
34.03526	0.067862
13.20408	0.166982
5.385013	0.313321
2.273935	0.379737
0.968280	0.191116
0.262790	0.011671
0.117605	−0.003700
0.049884	0.000778
	p space
Exponent	2p
	−0.240923
3.618910	0.029115
0.710985	0.169382
0.195089	0.513487
0.060176	0.479298

Table XLIII. Be ^3P $(13s5p)$ basis set, orbital energies and eigenvectors. Energy(E_H) = -14.511351

	s space
Exponent	1s
	-4.743702
29809.33	0.000038
4465.261	0.000293
1016.203	0.001537
287.7944	0.006432
93.85972	0.022729
33.84670	0.068282
13.12980	0.167859
5.353698	0.314445
2.259853	0.379585
0.961749	0.189042
0.258199	0.011154
0.114169	-0.003571
0.048510	0.000767

	p space
Exponent	2p
	-0.241366
7.435519	0.010741
1.576620	0.062866
0.435216	0.248127
0.143830	0.523680
0.049935	0.353506

Table XLIV. Be ^3P $(13s6p)$ basis set, orbital energies and eigenvectors. Energy$(E_H) = -14.511451$

	s space
Exponent	1s
	−4.743669
29717.43	0.000038
4451.500	0.000294
1013.072	0.001543
286.9084	0.006456
93.57136	0.022813
33.74325	0.068513
13.08996	0.168314
5.337896	0.314910
2.253707	0.379299
0.959305	0.188212
0.255794	0.010999
0.112910	−0.003575
0.048085	0.000777
	p space
Exponent	2p
	−0.241466
14.03416	0.004098
3.168386	0.025630
0.902416	0.103770
0.303551	0.311697
0.112972	0.498047
0.042857	0.258809

Table XLV. Be ^3P $(13s7p)$ basis set, orbital energies and eigenvectors. Energy(E_H) $= -14.511475$

	s space
Exponent	1s
	−4.743664
29734.32	0.000038
4454.029	0.000294
1013.647	0.001542
287.0712	0.006451
93.62442	0.022798
33.76235	0.068470
13.09745	0.168226
5.340861	0.314826
2.254819	0.379363
0.959688	0.188369
0.255887	0.011020
0.112960	−0.003582
0.048095	0.000779

	p space
Exponent	2p
	−0.241489
25.16644	0.001598
5.865884	0.011063
1.758030	0.044757
0.597307	0.148936
0.228295	0.355004
0.092574	0.453119
0.037674	0.188913

Table XLVI. Be ^3P $(13s8p)$ basis set, orbital energies and eigenvectors. Energy(E_H) $= -14.511481$

	s space
Exponent	1s
	−4.743664
29730.82	0.000038
4453.506	0.000294
1013.528	0.001542
287.0376	0.006453
93.61345	0.022801
33.75835	0.068479
13.09583	0.168245
5.340240	0.314841
2.254598	0.379348
0.959622	0.188337
0.255942	0.011017
0.112983	−0.003578
0.048100	0.000777
	p space
Exponent	2p
	−0.241495
43.74866	0.000634
10.33139	0.004806
3.226238	0.020534
1.127085	0.067797
0.433364	0.192958
0.180803	0.378565
0.078273	0.400640
0.033724	0.138049

Table XLVII. Be ^3P $(13s9p)$ basis set, orbital energies and eigenvectors. Energy(E_H) = −14.511482

	s space
Exponent	1s
	−4.743664
29731.67	0.000038
4453.632	0.000294
1013.557	0.001542
287.0458	0.006452
93.61613	0.022800
33.75937	0.068476
13.09624	0.168241
5.340380	0.314839
2.254642	0.379352
0.959634	0.188344
0.255933	0.011018
0.112978	−0.003579
0.048097	0.000778

	p space
Exponent	2p
	−0.241497
74.12825	0.000257
17.57599	0.002087
5.616600	0.009698
2.033661	0.032189
0.792249	0.094017
0.333857	0.231403
0.148658	0.385641
0.067782	0.347775
0.030612	0.101190

Table XLVIII. Be ^3P $(14s9p)$ basis set, orbital energies and eigenvectors. Energy$(E_H) = -14.511493$

	s space
Exponent	1s
	−4.743671
57979.96	0.000016
8683.343	0.000128
1976.123	0.000671
559.6980	0.002821
182.5772	0.010135
65.89918	0.031764
25.67140	0.085766
10.58415	0.190524
4.541691	0.323452
2.007203	0.350680
0.889418	0.156311
0.252558	0.008212
0.110214	−0.002372
0.047175	0.000473

	p space
Exponent	2p
	−0.241498
74.13232	0.000257
17.57659	0.002087
5.617012	0.009696
2.034151	0.032173
0.792459	0.094012
0.333831	0.231492
0.148646	0.385550
0.067790	0.347770
0.030612	0.101223

Table XLIX. Be ^3P $(15s9p)$ basis set, orbital energies and eigenvectors. Energy$(E_H) = -14.511497$

	s space
Exponent	1s
	−4.743674
107411.7	0.000008
16084.40	0.000059
3660.393	0.000311
1036.789	0.001311
338.2444	0.004742
122.1176	0.015183
47.62995	0.043088
19.73234	0.105831
8.556171	0.213843
3.839146	0.328552
1.770756	0.316408
0.817187	0.124577
0.248872	0.005893
0.107972	−0.001485
0.046456	0.000249

	p space
Exponent	2p
	−0.241498
74.17141	0.000257
17.58548	0.002086
5.619781	0.009689
2.035275	0.032151
0.792731	0.094014
0.333838	0.231524
0.148658	0.385456
0.067803	0.347816
0.030613	0.101269

Table L. Be ^3P $(16s9p)$ basis set, orbital energies and eigenvectors. Energy(E_H) = -14.511499

	s space
Exponent	1s
	-4.743675
171927.3	0.000004
25737.73	0.000033
5856.501	0.000173
1658.756	0.000729
541.1532	0.002649
195.3756	0.008558
76.21273	0.024865
31.60740	0.064188
13.75625	0.142226
6.210480	0.255412
2.892354	0.335226
1.387870	0.252108
0.672920	0.070358
0.238000	0.002462
0.103399	-0.000423
0.045087	-0.000008

	p space
Exponent	2p
	-0.241499
74.08562	0.000258
17.56670	0.002089
5.614891	0.009699
2.033692	0.032185
0.791862	0.094175
0.333480	0.231658
0.148577	0.385274
0.067788	0.347723
0.030603	0.101207

Table LI. Be ^3P $(17s10p)$ basis set, orbital energies and eigenvectors. Energy(E_H) $= -14.511501$

	s space
Exponent	1s
	−4.743676
244431.5	0.000003
36596.38	0.000021
8327.939	0.000111
2358.815	0.000470
769.5426	0.001710
277.8218	0.005551
108.3621	0.016314
44.93934	0.043268
19.57204	0.101033
8.846533	0.198784
4.107699	0.307710
1.946719	0.318777
0.922828	0.152806
0.357691	0.013919
0.179898	−0.002367
0.084785	0.000669
0.039595	−0.000229

	p space
Exponent	2p
	−0.241500
123.2720	0.000107
29.23626	0.000906
9.446704	0.004552
3.515753	0.015938
1.402691	0.045930
0.594170	0.121973
0.268091	0.262154
0.125788	0.379271
0.059919	0.298673
0.028113	0.074899

Table LII. B ^2P ($13s8p$) basis set. Energy(E_H) = -24.529017

	s space	
Exponent	1s	2s
	−7.695309	−0.494689
46535.63	0.000038	−0.000008
6970.783	0.000298	−0.000060
1586.432	0.001565	−0.000318
449.3104	0.006548	−0.001320
146.5617	0.023140	−0.004772
52.88387	0.069618	−0.014449
20.55825	0.171198	−0.038302
8.434628	0.319128	−0.077955
3.607517	0.374441	−0.133983
1.567314	0.181154	−0.102752
0.459387	0.010919	0.281268
0.183777	−0.002326	0.584616
0.072352	0.000695	0.275055

	p space
Exponent	2p
	−0.309839
69.07083	0.000785
16.31631	0.006056
5.115536	0.026894
1.821835	0.089865
0.713452	0.223722
0.292123	0.372919
0.121145	0.376246
0.049631	0.138621

Table LIII. B ^2P $(14s9p)$ basis set. Energy$(E_H) = -24.529040$

	s space	
Exponent	1s	2s
	−7.695320	−0.494696
80154.53	0.000020	−0.000004
12004.70	0.000151	−0.000031
2732.008	0.000795	−0.000160
773.7937	0.003339	−0.000679
252.4266	0.011975	−0.002424
91.12274	0.037325	−0.007755
35.51074	0.099610	−0.021041
14.66253	0.215509	−0.049825
6.332447	0.344358	−0.090515
2.849485	0.322651	−0.136107
1.311156	0.115699	−0.064657
0.436826	0.005342	0.311524
0.174889	−0.000633	0.576689
0.069996	0.000252	0.252168

	p space
Exponent	2p
	−0.309847
116.5023	0.000321
27.61730	0.002627
8.835726	0.012516
3.224158	0.043272
1.282857	0.122094
0.544011	0.255787
0.236298	0.370919
0.103490	0.326066
0.044645	0.101891

Table LIV. B ^2P $(15s10p)$ basis set. Energy$(E_H) = -24.529052$

	s space	
Exponent	1s	2s
	−7.695328	−0.494704
115192.9	0.000012	−0.000002
17250.75	0.000096	−0.000019
3925.815	0.000505	−0.000102
1111.915	0.002129	−0.000431
362.7114	0.007676	−0.001558
130.9140	0.024325	−0.004990
51.01528	0.067401	−0.014131
21.07452	0.157452	−0.034741
9.082244	0.290057	−0.071099
4.039391	0.363843	−0.117983
1.820917	0.217878	−0.125437
0.716189	0.027031	0.058299
0.332214	−0.003077	0.395662
0.143223	0.001280	0.510877
0.061637	−0.000237	0.173219

	p space
Exponent	2p
	−0.309854
192.4922	0.000135
45.64719	0.001147
14.75276	0.005848
5.503329	0.021167
2.222352	0.062659
0.959102	0.153006
0.431468	0.277961
0.196905	0.358966
0.090330	0.279446
0.040672	0.075356

Table LV. B ^2P $(16s11p)$ basis set. Energy$(E_H) = -24.529057$

	s space	
Exponent	1s	2s
	−7.695332	−0.494705
210307.5	0.000006	−0.000001
31490.56	0.000045	−0.000009
7166.350	0.000238	−0.000048
2029.835	0.001006	−0.000203
662.2068	0.003648	−0.000740
239.0604	0.011744	−0.002387
93.22870	0.033807	−0.006987
38.63073	0.085609	−0.018124
16.77308	0.182654	−0.041247
7.539163	0.305850	−0.077814
3.480558	0.340893	−0.121311
1.617179	0.175165	−0.108324
0.626869	0.017196	0.110166
0.293382	−0.002320	0.419394
0.130945	0.001019	0.472500
0.058144	−0.000185	0.142795

	p space
Exponent	2p
	−0.309855
312.4784	0.000058
74.06287	0.000506
24.03484	0.002722
9.095995	0.010466
3.741667	0.031864
1.632107	0.083911
0.749344	0.180095
0.353160	0.291538
0.167958	0.341076
0.080132	0.237524
0.037442	0.056023

Table LVI. B ^2P $(17s12p)$ basis set. Energy$(E_H) = -24.529059$

	s space	
Exponent	1s	2s
	−7.695333	−0.494705
379199.2	0.000003	−0.000001
56775.98	0.000022	−0.000004
12920.48	0.000114	−0.000023
3659.782	0.000482	−0.000097
1194.038	0.001754	−0.000354
431.1031	0.005693	−0.001157
168.1652	0.016738	−0.003413
69.75545	0.044419	−0.009249
30.39920	0.103895	−0.022259
13.76650	0.204393	−0.047234
6.422073	0.313360	−0.083155
3.068975	0.313013	−0.121493
1.471705	0.141319	−0.091631
0.587524	0.011952	0.141134
0.273510	−0.001347	0.432038
0.124157	0.000681	0.448526
0.056105	−0.000111	0.126072

	p space
Exponent	2p
	−0.309856
499.1207	0.000026
118.2240	0.000227
38.41494	0.001266
14.65022	0.005163
6.123082	0.016414
2.705304	0.044488
1.254685	0.105714
0.604595	0.202517
0.296145	0.297990
0.145949	0.319397
0.072029	0.200749
0.034757	0.041880

Table LVII. B ^2P $(18s13p)$ basis set. Energy$(E_H) = -24.529060$

	s space	
Exponent	1s	2s
	−7.695334	−0.494705
653630.4	0.000001	0.000000
97866.53	0.000011	−0.000002
22272.78	0.000058	−0.000012
6309.404	0.000244	−0.000049
2058.723	0.000890	−0.000180
743.3892	0.002900	−0.000586
290.0274	0.008618	−0.001755
120.3456	0.023466	−0.004808
52.51517	0.057873	−0.012159
23.87294	0.125511	−0.027317
11.20685	0.227706	−0.054143
5.402514	0.316970	−0.089117
2.664915	0.277894	−0.120034
1.319498	0.106757	−0.070881
0.553028	0.007662	0.169158
0.257238	−0.000519	0.440663
0.118510	0.000381	0.426487
0.054369	−0.000044	0.112463

	p space
Exponent	2p
	−0.309856
850.5789	0.000010
199.8506	0.000092
64.65040	0.000530
24.62523	0.002304
10.34207	0.007881
4.608119	0.022321
2.139967	0.056200
1.035154	0.123373
0.515352	0.217665
0.259484	0.299034
0.131286	0.299624
0.066437	0.173848
0.032832	0.032971

Table LVIII. C ^3P $(13s8p)$ basis set. Energy$(E_H) = -37.688543$

	s space	
Exponent	1s	2s
	−11.325480	−0.705598
67087.66	0.000039	−0.000008
10049.36	0.000301	−0.000064
2287.065	0.001579	−0.000338
647.7452	0.006609	−0.001407
211.2917	0.023367	−0.005088
76.24842	0.070422	−0.015460
29.66119	0.173606	−0.041228
12.19908	0.322922	−0.084527
5.244382	0.371572	−0.143127
2.296669	0.174922	−0.096027
0.712776	0.011357	0.294474
0.280890	−0.001686	0.582242
0.108589	0.000607	0.269801

	p space
Exponent	2p
	−0.433311
106.2282	0.000828
25.11938	0.006510
7.927761	0.029702
2.859484	0.098904
1.128484	0.236627
0.462328	0.375242
0.189933	0.362258
0.076140	0.132855

Table LIX. C ^3P $(14s9p)$ basis set. Energy$(E_H) = -37.688585$

	s space	
Exponent	1s	2s
	−11.325500	−0.705615
106825.5	0.000022	−0.000005
15999.46	0.000168	−0.000036
3641.109	0.000885	−0.000188
1031.249	0.003715	−0.000796
336.3831	0.013309	−0.002851
121.3999	0.041380	−0.009081
47.27937	0.109776	−0.024737
19.49560	0.234440	−0.058080
8.400201	0.360565	−0.105705
3.756462	0.303731	−0.145482
1.706644	0.084298	−0.031630
0.641466	0.002824	0.344968
0.256641	0.000423	0.561978
0.102375	0.000052	0.231163

	p space
Exponent	2p
	−0.433328
178.8735	0.000339
42.40502	0.002806
13.60687	0.013699
5.008865	0.048244
2.013259	0.133419
0.857530	0.267434
0.372058	0.368572
0.161262	0.311507
0.068124	0.097329

Table LX. C ^3P $(15s10p)$ basis set. Energy$(E_H) = -37.688605$

	s space	
Exponent	1s	2s
	−11.325510	−0.705624
171077.6	0.000012	−0.000003
25619.75	0.000093	−0.000020
5830.397	0.000491	−0.000105
1651.363	0.002070	−0.000442
538.6851	0.007469	−0.001600
194.4311	0.023708	−0.005136
75.77583	0.065968	−0.014605
31.32336	0.155303	−0.036302
13.52463	0.288755	−0.075222
6.033348	0.364257	−0.125625
2.727956	0.219975	−0.126764
1.087240	0.028832	0.076157
0.497943	−0.002508	0.409025
0.213993	0.001365	0.496338
0.091149	−0.000213	0.164143

	p space
Exponent	2p
	−0.433337
295.1695	0.000143
69.98253	0.001220
22.64185	0.006336
8.486302	0.023513
3.459493	0.069893
1.504280	0.165417
0.678384	0.287173
0.308658	0.352863
0.139995	0.265242
0.061791	0.071759

Table LXI. C ^3P $(16s11p)$ basis set. Energy$(E_H) = -37.688613$

	s space	
Exponent	1s	2s
	−11.325510	−0.705626
312229.0	0.000006	−0.000001
46749.69	0.000044	−0.000009
10638.55	0.000232	−0.000050
3013.287	0.000979	−0.000208
983.0464	0.003550	−0.000760
354.8877	0.011439	−0.002454
138.4034	0.033002	−0.007202
57.36184	0.083996	−0.018795
24.92838	0.180684	−0.043249
11.22964	0.304989	−0.082621
5.201549	0.341288	−0.128518
2.426564	0.177274	−0.107650
0.967344	0.018922	0.124086
0.445599	−0.001704	0.428463
0.197122	0.001032	0.461253
0.086347	−0.000151	0.137644

	p space
Exponent	2p
	−0.433339
478.6415	0.000062
113.4184	0.000537
36.81623	0.002926
13.96492	0.011503
5.780787	0.035720
2.543594	0.093119
1.173779	0.192644
0.553675	0.297782
0.262173	0.331927
0.123617	0.224215
0.056671	0.053226

Table LXII. C ^3P $(17s12p)$ basis set. Energy$(E_H) = -37.688616$

	s space	
Exponent	1s	2s
	−11.325520	−0.705627
557537.1	0.000003	−0.000001
83489.22	0.000021	−0.000005
19001.47	0.000112	−0.000024
5382.629	0.000475	−0.000101
1756.230	0.001726	−0.000368
634.1076	0.005604	−0.001202
247.3618	0.016495	−0.003551
102.6131	0.043877	−0.009651
44.73171	0.103123	−0.023381
20.27802	0.204185	−0.050115
9.481142	0.314054	−0.089082
4.545630	0.312285	−0.128379
2.189381	0.140839	−0.087798
0.901115	0.012970	0.156553
0.414666	−0.000788	0.439138
0.186604	0.000681	0.436630
0.083219	−0.000077	0.121310

	p space
Exponent	2p
	−0.433340
765.4553	0.000027
180.8628	0.000241
58.71441	0.001357
22.41625	0.005620
9.406214	0.018267
4.187198	0.050019
1.955876	0.116408
0.945336	0.214466
0.462763	0.301170
0.226796	0.308042
0.110592	0.188478
0.052400	0.039621

Table LXIII. C ^3P $(18s13p)$ basis set. Energy$(E_H) = -37.688618$

	s space	
Exponent	1s	2s
	−11.325520	−0.705627
949028.8	0.000001	0.000000
142083.0	0.000011	−0.000002
32332.47	0.000058	−0.000012
9158.117	0.000244	−0.000052
2987.909	0.000891	−0.000190
1078.788	0.002903	−0.000620
420.8308	0.008631	−0.001855
174.6003	0.023529	−0.005092
76.18292	0.058161	−0.012917
34.63588	0.126624	−0.029230
16.27076	0.230465	−0.058414
7.855479	0.319297	−0.096655
3.882172	0.274295	−0.126065
1.928334	0.102252	−0.061722
0.835806	0.007862	0.188828
0.386291	0.000007	0.446118
0.176860	0.000369	0.411333
0.080252	−0.000012	0.106552

	p space
Exponent	2p
	−0.433340
1147.619	0.000013
272.8695	0.000118
89.08207	0.000669
34.24945	0.002862
14.54532	0.009693
6.573601	0.027334
3.107697	0.067339
1.527390	0.140180
0.768646	0.231880
0.389539	0.298239
0.197324	0.280657
0.099364	0.155688
0.048587	0.029071

Table LXIV. N ^4S ($13s8p$) basis set. Energy(E_H) = -54.400811

	s space	
Exponent	1s	2s
	−15.629000	−0.945278
90867.87	0.000039	−0.000009
13611.53	0.000305	−0.000067
3097.754	0.001600	−0.000355
877.3470	0.006698	−0.001475
286.1847	0.023690	−0.005337
103.2779	0.071455	−0.016259
40.19030	0.176326	−0.043504
16.55353	0.326774	−0.089597
7.137857	0.368943	−0.149205
3.141175	0.168584	−0.089092
1.010765	0.011399	0.305380
0.394659	−0.001193	0.579267
0.150795	0.000539	0.264855

	p space
Exponent	2p
	−0.567543
150.0595	0.000861
35.50297	0.006847
11.25080	0.031760
4.089839	0.105330
1.621185	0.245201
0.663821	0.376146
0.270740	0.352969
0.106811	0.129274

Table LXV. N ^4S ($14s9p$) basis set. Energy(E_H) = -54.400883

	s space	
Exponent	1s	2s
	−15.629030	−0.945308
139911.3	0.000023	−0.000005
20955.07	0.000178	−0.000039
4768.892	0.000935	−0.000206
1350.644	0.003926	−0.000870
440.5458	0.014055	−0.003121
158.9715	0.043661	−0.009914
61.89354	0.115537	−0.027123
25.50873	0.245177	−0.063442
10.97703	0.368721	−0.115840
4.876508	0.292329	−0.148856
2.153146	0.068452	−0.005443
0.866822	0.001175	0.368361
0.348696	0.001011	0.546914
0.139167	−0.000052	0.214544

	p space
Exponent	2p
	−0.567572
252.2943	0.000353
59.81055	0.002942
19.22564	0.014582
7.115873	0.051889
2.877877	0.141345
1.228714	0.274859
0.532208	0.366399
0.228841	0.301971
0.095184	0.094504

Table LXVI. N ^4S $(15s10p)$ basis set. Energy$(E_H) = -54.400914$

	s space	
Exponent	1s	2s
	−15.629050	−0.945319
237311.0	0.000012	−0.000003
35538.08	0.000092	−0.000020
8087.507	0.000484	−0.000107
2290.645	0.002037	−0.000450
747.2224	0.007352	−0.001628
269.7010	0.023359	−0.005236
105.1182	0.065170	−0.014933
43.47125	0.154188	−0.037382
18.79426	0.288256	−0.078092
8.401602	0.364345	−0.130664
3.806280	0.220701	−0.126789
1.529810	0.029964	0.088240
0.694518	−0.002051	0.416831
0.297396	0.001410	0.486753
0.125625	−0.000193	0.158706

	p space
Exponent	2p
	−0.567584
415.8107	0.000149
98.57174	0.001277
31.91031	0.006707
11.99559	0.025269
4.918808	0.075165
2.148297	0.173985
0.969683	0.292820
0.439918	0.348237
0.197835	0.255934
0.086046	0.069523

Table LXVII. N ^4S $(16s11p)$ basis set. Energy$(E_H) = -54.400926$

	s space	
Exponent	1s	2s
	−15.629060	−0.945322
432381.1	0.000006	−0.000001
64743.42	0.000044	−0.000010
14733.70	0.000229	−0.000050
4173.254	0.000965	−0.000213
1361.477	0.003500	−0.000775
491.5049	0.011284	−0.002504
191.6857	0.032599	−0.007362
79.45499	0.083230	−0.019286
34.54968	0.179930	−0.044699
15.58673	0.304955	−0.086048
7.235444	0.341159	−0.133249
3.383739	0.177643	−0.106068
1.369728	0.019923	0.134480
0.625089	−0.001249	0.433822
0.274819	0.001041	0.453151
0.119209	−0.000127	0.134123

	p space
Exponent	2p
	−0.567587
673.5556	0.000064
159.5845	0.000562
51.80170	0.003085
19.67343	0.012298
8.175345	0.038625
3.616131	0.099815
1.673414	0.201185
0.789246	0.301309
0.372339	0.325325
0.174038	0.215452
0.078681	0.051455

Table LXVIII. N ^4S $(17s12p)$ basis set. Energy$(E_H) = -54.400931$

	s space	
Exponent	1s	2s
	−15.629060	−0.945323
767205.8	0.000003	−0.000001
114872.2	0.000021	−0.000005
26141.87	0.000112	−0.000025
7404.934	0.000472	−0.000104
2415.971	0.001716	−0.000378
872.2905	0.005573	−0.001236
340.2683	0.016411	−0.003656
141.1540	0.043719	−0.009954
61.54181	0.103056	−0.024222
27.91586	0.204796	−0.052253
13.07082	0.315093	−0.093373
6.279022	0.311129	−0.132751
3.031985	0.139308	−0.083665
1.269373	0.013475	0.168291
0.580212	−0.000378	0.443197
0.259608	0.000681	0.427704
0.114711	−0.000055	0.117789

	p space
Exponent	2p
	−0.567588
1094.960	0.000028
258.6611	0.000245
83.85255	0.001392
31.96225	0.005859
13.41121	0.019414
5.985471	0.053600
2.803630	0.123196
1.355736	0.221568
0.662396	0.302410
0.322912	0.300985
0.155921	0.181794
0.072820	0.038741

Table LXIX. N ^4S $(18s13p)$ basis set. Energy$(E_H) = -54.400933$

	s space	
Exponent	1s	2s
	−15.629060	−0.945323
1296296.	0.000001	0.000000
194068.6	0.000011	−0.000002
44160.57	0.000058	−0.000013
12507.72	0.000245	−0.000054
4080.476	0.000893	−0.000197
1473.140	0.002913	−0.000643
574.6066	0.008664	−0.001926
238.3700	0.023635	−0.005295
103.9936	0.058518	−0.013459
47.27944	0.127729	−0.030613
22.21871	0.232874	−0.061511
10.73569	0.321117	−0.102006
5.308856	0.271317	−0.129501
2.639177	0.098531	−0.053703
1.165764	0.007889	0.202976
0.537091	0.000370	0.448576
0.244904	0.000364	0.400312
0.110271	0.000007	0.102453

	p space
Exponent	2p
	−0.567588
1570.277	0.000015
373.3040	0.000129
121.9628	0.000733
46.96009	0.003143
19.99323	0.010720
9.076143	0.030419
4.318022	0.074237
2.133179	0.150181
1.076317	0.239622
0.545664	0.296696
0.275678	0.269602
0.137926	0.146406
0.066745	0.027362

Table LXX. O ^3P $(13s8p)$ basis set. Energy$(E_H) = -74.809202$

	s space	
Exponent	1s	2s
	−20.668560	−1.244241
117967.1	0.000040	−0.000009
17670.89	0.000309	−0.000070
4021.592	0.001621	−0.000370
1138.991	0.006786	−0.001539
371.5259	0.024004	−0.005569
134.0759	0.072440	−0.017002
52.18686	0.178830	−0.045590
21.51537	0.330182	−0.094219
9.295640	0.366684	−0.154545
4.105733	0.162987	−0.083374
1.358060	0.011223	0.317782
0.528574	−0.000829	0.577368
0.200111	0.000504	0.256699

	p space
Exponent	2p
	−0.631830
191.1178	0.000954
45.21729	0.007612
14.34992	0.035544
5.241780	0.116240
2.079045	0.257476
0.842664	0.373252
0.336108	0.341802
0.128626	0.129683

Table LXXI. O ^3P $(14s9p)$ basis set. Energy$(E_H) = -74.809322$

	s space	
Exponent	1s	2s
	−20.668610	−1.244291
180242.7	0.000023	−0.000005
26995.77	0.000182	−0.000041
6143.609	0.000956	−0.000217
1739.979	0.004015	−0.000915
567.5251	0.014375	−0.003290
204.7817	0.044657	−0.010441
79.72475	0.118149	−0.028680
32.86046	0.250258	−0.067084
14.14016	0.372278	−0.122867
6.262833	0.286495	−0.150937
2.710958	0.061794	0.012549
1.129117	0.000340	0.386637
0.457092	0.001313	0.535121
0.181990	−0.000082	0.200136

	p space
Exponent	2p
	−0.631881
320.1033	0.000393
75.88003	0.003285
24.39731	0.016371
9.053842	0.058348
3.675606	0.154364
1.565309	0.283941
0.669728	0.359460
0.281699	0.291939
0.113943	0.095003

Table LXXII. O ^3P $(15s10p)$ basis set. Energy$(E_H) = -74.809369$

	s space	
Exponent	1s	2s
	−20.668640	−1.244307
313953.3	0.000012	−0.000003
47015.27	0.000091	−0.000021
10699.38	0.000478	−0.000108
3030.408	0.002015	−0.000458
988.5364	0.007277	−0.001659
356.8013	0.023138	−0.005342
139.0734	0.064676	−0.015265
57.53144	0.153548	−0.038413
24.89720	0.288099	−0.080721
11.14726	0.364370	−0.135192
5.058184	0.220921	−0.127306
2.044093	0.030620	0.098907
0.924416	−0.001774	0.426480
0.395221	0.001444	0.477899
0.165476	−0.000164	0.151402

	p space
Exponent	2p
	−0.631898
525.7638	0.000167
124.6306	0.001433
40.34300	0.007548
15.17831	0.028601
6.245039	0.084362
2.732624	0.187427
1.227200	0.297954
0.549190	0.338622
0.241776	0.247235
0.102505	0.070022

Table LXXIII. O ^3P $(16s11p)$ basis set. Energy$(E_H) = -74.809387$

	s space	
Exponent	1s	2s
	−20.668650	−1.244311
570979.8	0.000005	−0.000001
85496.90	0.000043	−0.000010
19456.65	0.000227	−0.000051
5511.030	0.000957	−0.000217
1797.919	0.003472	−0.000791
649.0677	0.011196	−0.002559
253.1386	0.032375	−0.007530
104.9379	0.082835	−0.019782
45.65036	0.179668	−0.046086
20.61762	0.305201	−0.089189
9.586759	0.340889	−0.137550
4.492510	0.177421	−0.105109
1.836943	0.020470	0.144784
0.834803	−0.000959	0.441597
0.365722	0.001053	0.444545
0.157034	−0.000096	0.128232

	p space
Exponent	2p
	−0.631903
848.8125	0.000072
201.1044	0.000634
65.27654	0.003484
24.79467	0.013949
10.32060	0.043929
4.579817	0.111234
2.118986	0.213536
0.992587	0.302401
0.461596	0.314183
0.211411	0.208157
0.093349	0.051923

Table LXXIV. O ^3P $(17s12p)$ basis set. Energy$(E_H) = -74.809393$

	s space	
Exponent	1s	2s
	−20.668650	−1.244313
1007399.	0.000003	−0.000001
150832.4	0.000021	−0.000005
34324.73	0.000112	−0.000025
9722.658	0.000471	−0.000107
3172.127	0.001714	−0.000389
1145.291	0.005568	−0.001272
446.7586	0.016402	−0.003763
185.3304	0.043737	−0.010259
80.81104	0.103293	−0.025043
36.67349	0.205701	−0.054269
17.18953	0.316174	−0.097291
8.269773	0.309893	−0.136714
4.001779	0.137481	−0.080340
1.695655	0.013636	0.180130
0.773124	−0.000104	0.449703
0.344720	0.000685	0.417944
0.150796	−0.000026	0.112030

	p space
Exponent	2p
	−0.631905
1349.059	0.000032
319.4569	0.000286
103.7804	0.001616
39.62821	0.006785
16.66137	0.022499
7.464166	0.061674
3.509325	0.136845
1.695680	0.232485
0.822742	0.299822
0.395733	0.288243
0.187644	0.174557
0.085841	0.038726

Table LXXV. O ^3P $(18s13p)$ basis set. Energy$(E_H) = -74.809396$

	s space	
Exponent	1s	2s
	−20.668660	−1.244314
1678789.	0.000001	0.000000
251388.2	0.000011	−0.000002
57213.73	0.000059	−0.000013
16207.44	0.000249	−0.000056
5288.276	0.000907	−0.000206
1909.478	0.002957	−0.000672
744.9231	0.008791	−0.002013
309.0755	0.023980	−0.005535
134.8645	0.059381	−0.014079
61.33129	0.129650	−0.032113
28.83796	0.236064	−0.064676
13.94504	0.322921	−0.107154
6.899077	0.267395	−0.132438
3.431577	0.093843	−0.045655
1.539840	0.007533	0.218383
0.709751	0.000632	0.453380
0.323047	0.000356	0.387354
0.144222	0.000033	0.095865

	p space
Exponent	2p
	−0.631905
2113.513	0.000015
500.2799	0.000131
162.5448	0.000756
62.21343	0.003296
26.34014	0.011461
11.90574	0.033096
5.647594	0.080868
2.778214	0.159720
1.390190	0.245006
0.695281	0.292280
0.344642	0.262073
0.168538	0.145888
0.079551	0.029017

Table LXXVI. F ^2P ($13s8p$) basis set. Energy(E_H) = -99.409055

	s space	
Exponent	1s	2s
	−26.382630	−1.572426
148260.7	0.000040	−0.000009
22208.78	0.000313	−0.000072
5054.334	0.001642	−0.000382
1431.475	0.006874	−0.001591
466.9234	0.024317	−0.005756
168.5003	0.073402	−0.017604
65.59433	0.181205	−0.047270
27.05981	0.333292	−0.097913
11.70462	0.364663	−0.158320
5.180958	0.157878	−0.077772
1.748829	0.010977	0.327157
0.678763	−0.000532	0.575139
0.255259	0.000471	0.250726

	p space
Exponent	2p
	−0.729903
240.9728	0.001008
57.02125	0.008076
18.12833	0.037934
6.646791	0.122874
2.637797	0.264597
1.063762	0.371925
0.419292	0.334733
0.157487	0.128992

Table LXXVII. F ^2P ($14s9p$) basis set. Energy(E_H) = -99.409239

	s space	
Exponent	1s	2s
	-26.382700	-1.572501
227054.6	0.000024	-0.000005
34007.08	0.000184	-0.000043
7739.225	0.000966	-0.000224
2191.881	0.004056	-0.000943
714.9138	0.014521	-0.003392
257.9595	0.045123	-0.010765
100.4301	0.119447	-0.029663
41.40538	0.252950	-0.069469
17.82383	0.374032	-0.127467
7.884143	0.283163	-0.151737
3.372696	0.058671	0.025198
1.427030	-0.000010	0.397819
0.579525	0.001481	0.526415
0.230056	-0.000093	0.191036

	p space
Exponent	2p
	-0.729981
402.6951	0.000417
95.45520	0.003491
30.71017	0.017498
11.42608	0.062431
4.650914	0.162145
1.978158	0.289244
0.841147	0.355724
0.349553	0.285252
0.138942	0.094537

Table LXXVIII. F ^2P ($15s10p$) basis set. Energy(E_H) = -99.409308

	s space	
Exponent	1s	2s
	-26.382740	-1.572523
400745.7	0.000012	-0.000003
60013.08	0.000090	-0.000021
13657.40	0.000475	-0.000110
3868.237	0.002002	-0.000465
1261.848	0.007231	-0.001682
455.4532	0.023005	-0.005420
177.5331	0.064389	-0.015512
73.45899	0.153240	-0.039181
31.81364	0.288187	-0.082681
14.26084	0.364314	-0.138420
6.478246	0.220736	-0.127118
2.627737	0.031042	0.107000
1.184078	-0.001531	0.432627
0.505251	0.001465	0.471426
0.210080	-0.000144	0.146536

	p space
Exponent	2p
	-0.730005
660.0857	0.000177
156.4625	0.001526
50.65363	0.008071
19.08092	0.030741
7.872742	0.090101
3.449055	0.195337
1.544895	0.301021
0.686529	0.333179
0.298632	0.241177
0.124571	0.069702

Table LXXIX. F ^2P ($16s11p$) basis set. Energy(E_H) = -99.409333

	s space	
Exponent	1s	2s
	−26.382750	−1.572530
720491.5	0.000006	−0.000001
107968.2	0.000043	−0.000010
24588.99	0.000228	−0.000053
6969.674	0.000961	−0.000222
2275.306	0.003484	−0.000810
821.9317	0.011229	−0.002618
320.7533	0.032460	−0.007706
133.0541	0.083077	−0.020264
57.93265	0.180325	−0.047327
26.20134	0.306027	−0.091771
12.20503	0.339964	−0.140621
5.730828	0.175842	−0.103127
2.359605	0.020596	0.153799
1.068459	−0.000699	0.446806
0.466857	0.001050	0.437346
0.199023	−0.000074	0.123641

	p space
Exponent	2p
	−0.730012
1091.196	0.000074
257.8959	0.000652
83.52217	0.003611
31.67862	0.014612
13.18668	0.046366
5.855187	0.116552
2.704856	0.219163
1.260858	0.302939
0.581068	0.309139
0.262495	0.205238
0.113877	0.052825

Table LXXX. F ^2P $(17s12p)$ basis set. Energy$(E_H) = -99.409342$

	s space	
Exponent	1s	2s
	−26.382760	−1.572532
1277672.	0.000003	−0.000001
191300.7	0.000021	−0.000005
43534.31	0.000112	−0.000026
12331.35	0.000472	−0.000109
4023.248	0.001717	−0.000398
1452.587	0.005577	−0.001299
566.6280	0.016433	−0.003847
235.0575	0.043846	−0.010498
102.5020	0.103680	−0.025686
46.53321	0.206721	−0.055840
21.82785	0.317220	−0.100283
10.51179	0.308647	−0.139390
5.093690	0.135597	−0.076985
2.176174	0.013682	0.189153
0.989967	0.000119	0.453549
0.440127	0.000684	0.410711
0.191072	−0.000007	0.108063

	p space
Exponent	2p
	−0.730015
1687.718	0.000035
399.6517	0.000306
129.8267	0.001731
49.57826	0.007297
20.86193	0.024313
9.365564	0.066434
4.409977	0.144518
2.128376	0.238386
1.028288	0.298534
0.490757	0.281139
0.230073	0.169981
0.103766	0.038581

Table LXXXI. F ^2P $(18s13p)$ basis set. Energy$(E_H) = -99.409346$

	s space	
Exponent	1s	2s
	−26.382760	−1.572534
2115112.	0.000002	0.000000
316699.7	0.000011	−0.000003
72075.71	0.000060	−0.000014
20416.83	0.000251	−0.000058
6661.458	0.000916	−0.000212
2405.188	0.002987	−0.000693
938.2595	0.008882	−0.002075
389.2710	0.024232	−0.005710
169.8499	0.060031	−0.014536
77.24367	0.131135	−0.033235
36.32874	0.238563	−0.067066
17.57387	0.324308	−0.110984
8.693530	0.264376	−0.134146
4.321769	0.090284	−0.038741
1.959520	0.007258	0.229727
0.903185	0.000830	0.455729
0.410405	0.000350	0.377821
0.182024	0.000050	0.091345

	p space
Exponent	2p
	−0.730017
2641.133	0.000016
625.1424	0.000141
203.1062	0.000811
77.73855	0.003544
32.92397	0.012376
14.90071	0.035842
7.082732	0.086781
3.486351	0.167378
1.740970	0.249265
0.866502	0.289260
0.426099	0.254854
0.206097	0.142076
0.095982	0.028950

Table LXXXII. Ne ^1S $(13s8p)$ basis set. Energy$(E_H) = -128.546677$

	s space	
Exponent	1s	2s
	−128.546677	−32.772270
181825.6	0.000041	−0.000010
27236.69	0.000317	−0.000074
6198.592	0.001661	−0.000392
1755.538	0.006954	−0.001634
572.6181	0.024601	−0.005910
206.6382	0.074267	−0.018098
80.44709	0.183315	−0.048643
33.20103	0.335994	−0.100920
14.37044	0.362912	−0.161086
6.368538	0.153443	−0.072636
2.183540	0.010723	0.334401
0.845533	−0.000291	0.572841
0.316405	0.000441	0.246297

	p space
Exponent	2p
	−0.850252
298.6089	0.001041
70.67233	0.008377
22.50569	0.039540
8.275682	0.127244
3.286264	0.269217
1.321757	0.371272
0.517403	0.329867
0.191946	0.127985

Table LXXXIII. Ne ^1S $(14s9p)$ basis set. Energy$(E_H) = -128.546946$

	s space	
Exponent	1s	2s
	−32.772370	−1.930344
279982.9	0.000024	−0.000006
41934.54	0.000185	−0.000043
9543.344	0.000970	−0.000228
2702.837	0.004075	−0.000961
881.5658	0.014591	−0.003460
318.0896	0.045361	−0.010983
123.8462	0.120165	−0.030337
51.07396	0.254555	−0.071156
21.99610	0.375020	−0.130710
9.724086	0.281059	−0.152015
4.129984	0.057006	0.034434
1.761354	−0.000148	0.405064
0.716347	0.001585	0.519898
0.283574	−0.000098	0.185083

	p space
Exponent	2p
	−0.850359
498.2942	0.000431
118.1143	0.003622
38.02522	0.018251
14.17914	0.065179
5.782939	0.167231
2.458300	0.292729
1.041767	0.353479
0.429802	0.280484
0.168841	0.093773

Table LXXXIV. Ne ^1S $(15s10p)$ basis set. Energy$(E_H) = -128.547042$

	s space	
Exponent	1s	2s
	−32.772410	−1.930375
497852.4	0.000012	−0.000003
74555.06	0.000090	−0.000021
16966.77	0.000473	−0.000111
4805.560	0.001993	−0.000469
1567.610	0.007200	−0.001699
565.8163	0.022913	−0.005479
220.5583	0.064199	−0.015699
91.27878	0.153072	−0.039769
39.55424	0.288341	−0.084190
17.74704	0.364228	−0.140817
8.068670	0.220448	−0.126660
3.282109	0.031358	0.113186
1.474346	−0.001323	0.436635
0.627895	0.001479	0.466579
0.259676	−0.000130	0.143304

	p space
Exponent	2p
	−0.850393
815.7149	0.000184
193.3414	0.001585
62.60427	0.008415
23.61085	0.032195
9.763452	0.093942
4.281453	0.200489
1.915091	0.303107
0.847682	0.329744
0.366024	0.236716
0.150996	0.069115

Table LXXXV. Ne ^1S $(16s11p)$ basis set. Energy$(E_H) = -128.547076$

	s space	
Exponent	1s	2s
	−32.772430	−1.930384
902420.7	0.000005	−0.000001
135126.9	0.000043	−0.000010
30751.46	0.000225	−0.000053
8710.380	0.000950	−0.000223
2841.714	0.003448	−0.000814
1025.901	0.011125	−0.002632
400.1128	0.032205	−0.007759
165.8865	0.082616	−0.020457
72.20594	0.179890	−0.047972
32.65977	0.306072	−0.093406
15.21874	0.340132	−0.142784
7.149032	0.176128	−0.102257
2.957144	0.021033	0.158710
1.335145	−0.000517	0.449458
0.581579	0.001062	0.433493
0.246331	−0.000061	0.121576

	p space
Exponent	2p
	−0.850403
1312.610	0.000080
310.9703	0.000704
100.9378	0.003888
38.37623	0.015717
16.02832	0.049680
7.142050	0.122901
3.304475	0.225428
1.539370	0.303829
0.707459	0.303388
0.317896	0.198783
0.136812	0.051249

Table LXXXVI. Ne ^1S $(17s12p)$ basis set. Energy$(E_H) = -128.547089$

	s space	
Exponent	1s	2s
	−32.772440	−1.930388
1579098.	0.000003	−0.000001
236433.9	0.000021	−0.000005
53805.89	0.000112	−0.000026
15240.90	0.000473	−0.000111
4972.496	0.001720	−0.000404
1795.289	0.005588	−0.001321
700.2988	0.016469	−0.003913
290.5059	0.043964	−0.010685
126.6876	0.104058	−0.026193
57.52756	0.207647	−0.057079
27.00068	0.318120	−0.102620
13.01199	0.307552	−0.141275
6.310875	0.133951	−0.073944
2.712472	0.013696	0.196044
1.231615	0.000300	0.455789
0.546255	0.000683	0.405283
0.235804	0.000006	0.105380

	p space
Exponent	2p
	−0.850407
2080.586	0.000036
492.6660	0.000319
160.0345	0.001806
61.12231	0.007641
25.74117	0.025561
11.57601	0.069677
5.457011	0.149589
2.632106	0.242259
1.268597	0.297836
0.602693	0.276383
0.280519	0.166388
0.125270	0.038233

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Table LXXXVII. Ne ^1S $(18s13p)$ basis set. Energy$(E_H) = -128.547094$

	s space	
Exponent	1s	2s
	−32.772440	−1.930390
2598845.	0.000002	0.000000
389291.2	0.000011	−0.000003
88614.78	0.000060	−0.000014
25103.59	0.000254	−0.000060
8190.910	0.000924	−0.000217
2957.497	0.003012	−0.000709
1153.743	0.008955	−0.002123
478.6800	0.024435	−0.005845
208.8645	0.060551	−0.014889
94.99324	0.132322	−0.034108
44.68681	0.240541	−0.068931
21.62328	0.325338	−0.113917
10.69442	0.261968	−0.135140
5.311698	0.087551	−0.032906
2.426042	0.007054	0.238232
1.118112	0.000983	0.456691
0.507378	0.000345	0.370650
0.223960	0.000060	0.088250

	p space
Exponent	2p
	−0.850408
3257.313	0.000016
771.0460	0.000147
250.5331	0.000844
95.90373	0.003698
40.63348	0.012971
18.40949	0.037674
8.762468	0.090682
4.314311	0.172338
2.151501	0.252099
1.067635	0.287512
0.522400	0.250033
0.250843	0.139050
0.115708	0.028707

Table LXXXVIII. K ^2S $(20s12p)$ basis set. Energy$(E_H) = -599.164579$

		s space		
Exponent	$1s$	$2s$	$3s$	$4s$
	−133.533000	−14.489900	−1.748732	−0.147449
3552528.	0.000005	−0.000001	0.000001	0.000000
531942.2	0.000039	−0.000011	0.000004	−0.000001
121055.1	0.000205	−0.000059	0.000020	−0.000004
34288.69	0.000866	−0.000249	0.000082	−0.000016
11186.49	0.003146	−0.000908	0.000300	−0.000058
4038.519	0.010169	−0.002945	0.000969	−0.000187
1575.136	0.029571	−0.008714	0.002885	−0.000557
653.2363	0.076662	−0.023283	0.007695	−0.001488
284.7008	0.170140	−0.055730	0.018677	−0.003607
129.1997	0.297465	−0.112354	0.037918	−0.007358
60.55350	0.343659	−0.175577	0.061996	−0.012016
28.77402	0.192637	−0.131402	0.047400	−0.009333
12.43072	0.027680	0.192728	−0.076287	0.015228
5.984502	−0.001746	0.562457	−0.316527	0.064540
2.873281	0.001250	0.376937	−0.338098	0.073193
1.151932	−0.000534	0.041007	0.279340	−0.073883
0.536411	0.000227	−0.003174	0.687207	−0.177399
0.236797	−0.000085	0.001562	0.292588	−0.231067
0.038158	0.000017	−0.000217	0.004591	0.701712
0.016426	−0.000008	0.000102	−0.001213	0.433110

	p space	
Exponent	$2p$	$3p$
	−11.519200	−0.954377
3469.633	0.000213	−0.000065
822.0937	0.001863	−0.000568
266.6256	0.010205	−0.003136
101.2994	0.040775	−0.012661
42.43650	0.122522	−0.039183
18.91459	0.263991	−0.087049
8.702928	0.382237	−0.133982
4.086109	0.300080	−0.098717
1.867191	0.078095	0.152860
0.845487	0.001516	0.445829
0.368114	0.001087	0.438696
0.151710	−0.000249	0.128450

Table LXXXIX. K ^2S $(24s12p)$ basis set. Energy$(E_H) = -599.164627$

		s space		
Exponent	$1s$	$2s$	$3s$	$4s$
	−133.533000	−14.489910	−1.748748	−0.147451
14643700.	0.000001	0.000000	0.000000	0.000000
2192808.	0.000007	−0.000002	0.000001	0.000000
499186.1	0.000035	−0.000010	0.000003	−0.000001
141443.0	0.000148	−0.000042	0.000014	−0.000003
46161.77	0.000538	−0.000155	0.000051	−0.000010
16671.45	0.001758	−0.000506	0.000167	−0.000032
6504.751	0.005255	−0.001519	0.000501	−0.000097
2699.032	0.014519	−0.004228	0.001396	−0.000269
1177.878	0.037003	−0.010982	0.003629	−0.000701
536.1627	0.085550	−0.026333	0.008743	−0.001688
252.8131	0.172434	−0.057288	0.019150	−0.003706
122.7579	0.280892	−0.107863	0.036666	−0.007095
61.02093	0.318691	−0.161334	0.056445	−0.010985
30.64274	0.194407	−0.135660	0.049920	−0.009714
14.81984	0.039231	0.091051	−0.036685	0.007137
7.539629	−0.000086	0.443413	−0.212801	0.043083
3.876895	0.001421	0.472843	−0.364283	0.076963
1.988113	−0.000532	0.148008	−0.113354	0.023010
0.946278	0.000196	0.009146	0.445241	−0.111371
0.450778	−0.000131	0.001423	0.609855	−0.176715
0.211623	0.000035	0.000191	0.202291	−0.203533
0.043017	−0.000014	0.000025	0.003744	0.530277
0.021407	0.000013	−0.000025	−0.001641	0.521004
0.011095	−0.000004	0.000007	0.000593	0.096095

	p space	
Exponent	$2p$	$3p$
	−11.519220	−0.954389
3472.724	0.000213	−0.000065
822.8276	0.001860	−0.000567
266.8657	0.010190	−0.003132
101.3924	0.040718	−0.012644
42.47685	0.122373	−0.039133
18.93364	0.263761	−0.086973
8.712136	0.382138	−0.133923
4.090639	0.300352	−0.098923
1.869812	0.078343	0.152285
0.846593	0.001549	0.445666
0.368490	0.001084	0.439162
0.151813	−0.000248	0.128715

Table XC. K ^2S $(21s13p)$ basis set. Energy$(E_H) = -599.164704$

		s space		
Exponent	$1s$	$2s$	$3s$	$4s$
	−133.533000	−14.489930	−1.748754	−0.147462
6110612.	0.000002	−0.000001	0.000000	0.000000
914898.7	0.000020	−0.000006	0.000002	0.000000
208201.3	0.000104	−0.000030	0.000010	−0.000002
58973.96	0.000440	−0.000127	0.000042	−0.000008
19240.90	0.001603	−0.000461	0.000152	−0.000029
6946.875	0.005211	−0.001506	0.000498	−0.000096
2709.840	0.015392	−0.004479	0.001475	−0.000285
1124.193	0.041306	−0.012287	0.004073	−0.000786
490.4526	0.098858	−0.030592	0.010127	−0.001959
223.0501	0.200773	−0.068053	0.022896	−0.004424
105.0367	0.314241	−0.126244	0.042867	−0.008322
50.89952	0.312335	−0.174863	0.062500	−0.012130
24.99527	0.144198	−0.092204	0.033139	−0.006546
11.28001	0.016910	0.250622	−0.102059	0.020342
5.506071	−0.000380	0.560183	−0.332965	0.068441
2.698936	0.000554	0.327884	−0.302363	0.065323
1.118040	−0.000240	0.032946	0.314961	−0.081572
0.519406	0.000069	−0.001691	0.676740	−0.178680
0.231824	−0.000034	0.001153	0.274320	−0.225024
0.038439	0.000006	−0.000144	0.004184	0.696171
0.016531	−0.000003	0.000066	−0.001034	0.440323

	p space	
Exponent	$2p$	$3p$
	−11.519250	−0.954399
5394.492	0.000099	−0.000030
1277.631	0.000873	−0.000267
414.8357	0.004915	−0.001501
158.2664	0.020569	−0.006361
66.69915	0.067205	−0.021068
30.09624	0.167840	−0.054526
14.15178	0.303500	−0.101294
6.814214	0.366243	−0.132689
3.324985	0.226259	−0.049999
1.551104	0.043999	0.226704
0.715110	0.000337	0.457683
0.321040	0.000653	0.381272
0.135655	−0.000145	0.092901

Table XCI. K ^2S $(22s14p)$ basis set. Energy$(E_H) = -599.164751$

		s space		
Exponent	$1s$	$2s$	$3s$	$4s$
	−133.533000	−14.489940	−1.748767	−0.147468
9643537.	0.000001	0.000000	0.000000	0.000000
1443689.	0.000011	−0.000003	0.000001	0.000000
328535.9	0.000059	−0.000017	0.000006	−0.000001
93061.15	0.000249	−0.000072	0.000024	−0.000005
30363.00	0.000908	−0.000261	0.000086	−0.000017
10962.82	0.002961	−0.000853	0.000281	−0.000054
4276.521	0.008812	−0.002555	0.000844	−0.000163
1774.211	0.024089	−0.007066	0.002330	−0.000450
774.1564	0.059960	−0.018091	0.006003	−0.001159
352.2324	0.132052	−0.042103	0.013990	−0.002706
165.9201	0.242059	−0.086504	0.029244	−0.005656
80.45365	0.327710	−0.145597	0.050033	−0.009718
39.85383	0.261313	−0.166257	0.060401	−0.011751
19.85182	0.084539	−0.022183	0.007111	−0.001440
9.640847	0.005797	0.334442	−0.143548	0.028673
4.830961	0.001039	0.538904	−0.351508	0.073152
2.436275	−0.000182	0.255139	−0.239769	0.051357
1.064614	0.000052	0.022664	0.362833	−0.091950
0.496610	−0.000073	−0.000075	0.657785	−0.179389
0.225308	0.000012	0.000689	0.250556	−0.216736
0.038805	−0.000004	−0.000063	0.003719	0.689056
0.016665	0.000002	0.000027	−0.000841	0.449614

	p space	
Exponent	$2p$	$3p$
	−11.519260	−0.954411
8066.702	0.000049	−0.000015
1909.816	0.000436	−0.000133
620.3136	0.002493	−0.000763
237.1839	0.010796	−0.003313
100.3696	0.037199	−0.011582
45.55180	0.102664	−0.032646
21.70483	0.216363	−0.071208
10.63275	0.331509	−0.113023
5.317673	0.326149	−0.119733
2.679222	0.152360	0.012658
1.296957	0.021617	0.286862
0.611354	0.000566	0.453485
0.282062	0.000191	0.324807
0.121226	−0.000036	0.065641

Table XCII. K ^2S ($23s15p$) basis set. Energy(E_H) = -599.164771

	s space			
Exponent	$1s$	$2s$	$3s$	$4s$
	-133.533000	-14.489950	-1.748774	-0.147471
15243700.	0.000001	0.000000	0.000000	0.000000
2281775.	0.000006	-0.000002	0.000001	0.000000
519223.2	0.000033	-0.000010	0.000003	-0.000001
147070.8	0.000141	-0.000040	0.000013	-0.000003
47986.39	0.000513	-0.000148	0.000049	-0.000009
17327.54	0.001676	-0.000482	0.000159	-0.000031
6760.273	0.005011	-0.001448	0.000477	-0.000092
2805.143	0.013852	-0.004032	0.001331	-0.000257
1224.335	0.035359	-0.010480	0.003462	-0.000669
557.4206	0.082017	-0.025185	0.008362	-0.001616
262.9099	0.166455	-0.054991	0.018365	-0.003551
127.6980	0.274844	-0.104431	0.035476	-0.006871
63.50296	0.320131	-0.158768	0.055377	-0.010759
31.93999	0.204583	-0.141802	0.052114	-0.010174
15.62730	0.045221	0.066786	-0.027080	0.005323
7.961981	0.000500	0.417816	-0.194952	0.039181
4.104022	0.001437	0.488510	-0.360290	0.076158
2.117888	-0.000487	0.174615	-0.151845	0.031257
0.991996	0.000167	0.012814	0.413274	-0.102762
0.470524	-0.000116	0.001117	0.627888	-0.178584
0.218207	0.000026	0.000326	0.224773	-0.206900
0.039177	-0.000006	-0.000005	0.003313	0.682131
0.016796	0.000003	-0.000001	-0.000680	0.458809

	p space	
Exponent	$2p$	$3p$
	-11.519270	-0.954418
11795.98	0.000025	-0.000008
2791.905	0.000225	-0.000069
906.8900	0.001304	-0.000398
347.1443	0.005783	-0.001772
147.3445	0.020719	-0.006402
67.13126	0.061085	-0.019186
32.21743	0.144582	-0.046712
15.98942	0.261000	-0.086904
8.091286	0.340507	-0.119834
4.158564	0.267347	-0.091012
2.127531	0.090712	0.088700
1.062142	0.008391	0.336998
0.515042	0.000715	0.432475
0.244484	-0.000048	0.262820
0.106062	0.000013	0.042488

Table XCIII. K ^2S $(23s16p)$ basis set. Energy$(E_H) = -599.164776$

		s space		
Exponent	$1s$	$2s$	$3s$	$4s$
	0.000000	0.000000	0.000000	0.000000
15191300.	0.000001	0.000000	0.000000	0.000000
2275313.	0.000006	−0.000002	0.000001	0.000000
517929.9	0.000033	−0.000010	0.000003	−0.000001
146732.3	0.000141	−0.000041	0.000013	−0.000003
47883.44	0.000514	−0.000148	0.000049	−0.000009
17293.27	0.001680	−0.000483	0.000159	−0.000031
6748.149	0.005021	−0.001451	0.000478	−0.000092
2800.650	0.013876	−0.004039	0.001334	−0.000257
1222.597	0.035410	−0.010495	0.003467	−0.000670
556.7173	0.082113	−0.025216	0.008373	−0.001618
262.6129	0.166596	−0.055047	0.018383	−0.003555
127.5683	0.274958	−0.104501	0.035501	−0.006876
63.44479	0.320057	−0.158808	0.055394	−0.010763
31.91262	0.204353	−0.141661	0.052066	−0.010165
15.61080	0.045099	0.067199	−0.027248	0.005357
7.955703	0.000481	0.418038	−0.195119	0.039214
4.101871	0.001440	0.488133	−0.360195	0.076146
2.117504	−0.000489	0.174436	−0.151528	0.031178
0.991636	0.000168	0.012826	0.413404	−0.102783
0.470430	−0.000116	0.001107	0.627726	−0.178579
0.218188	0.000026	0.000329	0.224697	−0.206847
0.039174	−0.000006	−0.000005	0.003309	0.682227
0.016794	0.000003	−0.000001	−0.000677	0.458710

	p space	
Exponent	$2p$	$3p$
	0.000000	0.000000
17427.76	0.000013	−0.000004
4121.179	0.000114	−0.000035
1337.990	0.000668	−0.000204
512.2040	0.003018	−0.000924
217.7571	0.011171	−0.003433
99.51385	0.034590	−0.010766
47.96809	0.089307	−0.028358
24.04798	0.184148	−0.060292
12.34364	0.290481	−0.098052
6.439870	0.324973	−0.117681
3.392307	0.206546	−0.051432
1.758105	0.053386	0.155260
0.892205	0.003447	0.367548
0.442692	0.000556	0.402490
0.214830	−0.000070	0.209948
0.092907	0.000011	0.027203

Table XCIV. K ^2S ($24s15p$) basis set. Energy(E_H) = -599.164772

	s space			
Exponent	$1s$	$2s$	$3s$	$4s$
	-133.533000	-14.489950	-1.748775	-0.147473
14679730.	0.000001	0.000000	0.000000	0.000000
2198853.	0.000007	-0.000002	0.000001	0.000000
500578.8	0.000035	-0.000010	0.000003	-0.000001
141845.1	0.000147	-0.000042	0.000014	-0.000003
46298.45	0.000536	-0.000154	0.000051	-0.000010
16724.01	0.001751	-0.000504	0.000166	-0.000032
6527.125	0.005231	-0.001512	0.000498	-0.000096
2709.358	0.014444	-0.004206	0.001389	-0.000268
1182.946	0.036795	-0.010918	0.003608	-0.000697
538.7619	0.085043	-0.026169	0.008689	-0.001678
254.1912	0.171464	-0.056920	0.019023	-0.003682
123.5017	0.279762	-0.107254	0.036457	-0.007055
61.42636	0.318752	-0.160808	0.056227	-0.010946
30.86899	0.196106	-0.136732	0.050314	-0.009787
14.96913	0.040287	0.086248	-0.034793	0.006756
7.623109	0.000011	0.437947	-0.208902	0.042294
3.924917	0.001429	0.475880	-0.363332	0.076673
2.018044	-0.000524	0.153767	-0.121918	0.025048
0.955909	0.000190	0.009987	0.438642	-0.109941
0.454883	-0.000128	0.001332	0.613829	-0.176544
0.213104	0.000034	0.000227	0.206915	-0.205017
0.042674	-0.000013	0.000015	0.003836	0.541228
0.021068	0.000012	-0.000016	-0.001649	0.518138
0.010844	-0.000004	0.000004	0.000590	0.087256

	p space	
Exponent	$2p$	$3p$
	-11.519270	-0.954418
11776.80	0.000025	-0.000008
2787.538	0.000226	-0.000069
905.5880	0.001307	-0.000399
346.6905	0.005794	-0.001775
147.1676	0.020755	-0.006413
67.05671	0.061173	-0.019214
32.18398	0.144734	-0.046763
15.97347	0.261166	-0.086963
8.083416	0.340538	-0.119859
4.154545	0.267119	-0.090872
2.125356	0.090495	0.089068
1.061072	0.008349	0.337244
0.514577	0.000715	0.432325
0.244310	-0.000049	0.262479
0.106006	0.000013	0.042407

Table XCV. K ^2S $(25s16p)$ basis set. Energy$(E_H) = -599.164780$

		s space		
Exponent	$1s$	$2s$	$3s$	$4s$
	−133.533000	−14.489960	−1.748778	−0.147474
25145540.	0.000000	0.000000	0.000000	0.000000
3755894.	0.000003	−0.000001	0.000000	0.000000
852950.7	0.000018	−0.000005	0.000002	0.000000
241121.6	0.000076	−0.000022	0.000007	−0.000001
78511.16	0.000278	−0.000080	0.000026	−0.000005
28292.51	0.000911	−0.000262	0.000086	−0.000017
11017.83	0.002741	−0.000790	0.000260	−0.000050
4564.414	0.007649	−0.002216	0.000731	−0.000141
1989.526	0.019886	−0.005819	0.001921	−0.000371
904.9896	0.047822	−0.014331	0.004743	−0.000917
426.8215	0.104072	−0.032589	0.010833	−0.002093
207.5566	0.195833	−0.067091	0.022514	−0.004359
103.5820	0.292864	−0.118423	0.040445	−0.007833
52.76717	0.296414	−0.161987	0.057263	−0.011155
27.07669	0.156075	−0.108317	0.040062	−0.007801
13.24989	0.026091	0.146198	−0.059215	0.011607
6.811442	−0.000010	0.473502	−0.240531	0.048982
3.542858	0.000955	0.431127	−0.355606	0.075645
1.820014	−0.000358	0.113796	−0.056300	0.009705
0.895463	0.000116	0.005712	0.469362	−0.116786
0.433750	−0.000089	0.001657	0.584549	−0.175086
0.206792	0.000021	0.000083	0.185950	−0.197081
0.043699	−0.000008	0.000049	0.003381	0.513000
0.021839	0.000007	−0.000045	−0.001319	0.532714
0.011259	−0.000003	0.000014	0.000489	0.103667

	p space	
Exponent	$2p$	$3p$
	−11.519280	−0.954421
17375.31	0.000013	−0.000004
4109.439	0.000115	−0.000035
1334.363	0.000671	−0.000205
510.9001	0.003030	−0.000927
217.2493	0.011209	−0.003445
99.30562	0.034686	−0.010796
47.87831	0.089496	−0.028420
24.00612	0.184430	−0.060389
12.32187	0.290784	−0.098165
6.427428	0.324989	−0.117713
3.384675	0.206057	−0.050962
1.753106	0.052998	0.156429
0.889129	0.003385	0.368497
0.441014	0.000555	0.402039
0.214005	−0.000071	0.208569
0.092491	0.000011	0.026799

Table XCVI. Ca ^1S $(20s12p)$ basis set. Energy(E_H) = −676.757915

		s space		
Exponent	$1s$	$2s$	$3s$	$4s$
	−149.363600	−16.822680	−2.245327	−0.195506
2402654.	0.000009	−0.000003	0.000001	0.000000
359789.8	0.000072	−0.000021	0.000007	−0.000002
81878.09	0.000381	−0.000111	0.000038	−0.000009
23190.89	0.001604	−0.000467	0.000161	−0.000038
7565.212	0.005808	−0.001695	0.000585	−0.000140
2730.702	0.018596	−0.005483	0.001895	−0.000453
1064.640	0.052878	−0.015966	0.005525	−0.001320
441.0605	0.130151	−0.041514	0.014470	−0.003458
191.7269	0.259315	−0.092864	0.032716	−0.007836
86.53774	0.361496	−0.165317	0.060032	−0.014414
39.89924	0.264112	−0.176641	0.067016	−0.016215
17.64065	0.057094	0.064445	−0.025935	0.006345
8.359987	−0.001822	0.510879	−0.267477	0.067397
3.951330	0.002112	0.494638	−0.426964	0.114470
1.713396	−0.000977	0.087501	0.067949	−0.026356
0.810860	0.000456	−0.003591	0.710222	−0.233644
0.360247	−0.000191	0.002492	0.441783	−0.316106
0.081076	0.000092	−0.000757	0.021995	0.332837
0.044839	−0.000079	0.000645	−0.011936	0.561126
0.021429	0.000022	−0.000182	0.002656	0.280790

	p space	
Exponent	$2p$	$3p$
	−13.629190	−1.340659
4062.109	0.000198	−0.000065
962.4149	0.001732	−0.000565
312.2069	0.009533	−0.003131
118.7184	0.038392	−0.012743
49.80227	0.116792	−0.039922
22.25502	0.256354	−0.090550
10.28426	0.379854	−0.142607
4.859830	0.308067	−0.109889
2.252196	0.085763	0.151388
1.032869	0.002463	0.464069
0.460309	0.001010	0.437053
0.190111	−0.000253	0.107187

Table XCVII. Ca ^1S $(21s13p)$ basis set. Energy$(E_H) = -676.758079$

		s space		
Exponent	$1s$	$2s$	$3s$	$4s$
	−149.363700	−16.822720	−2.245354	−0.195519
4267399.	0.000005	−0.000001	0.000001	0.000000
638967.4	0.000035	−0.000010	0.000004	−0.000001
145409.4	0.000186	−0.000054	0.000019	−0.000004
41186.78	0.000784	−0.000228	0.000079	−0.000019
13436.89	0.002849	−0.000830	0.000287	−0.000068
4850.897	0.009219	−0.002697	0.000930	−0.000222
1891.922	0.026891	−0.007990	0.002765	−0.000661
784.5675	0.070191	−0.021470	0.007434	−0.001775
341.9075	0.158086	−0.051832	0.018138	−0.004341
155.1072	0.284466	−0.106696	0.037731	−0.009029
72.63168	0.347716	−0.172742	0.063460	−0.015289
34.49878	0.214838	−0.148928	0.056798	−0.013688
15.23646	0.036774	0.139354	−0.057671	0.013934
7.419390	−0.002032	0.538465	−0.302465	0.077408
3.597494	0.001663	0.428852	−0.391548	0.104532
1.562143	−0.000772	0.064089	0.154584	−0.050129
0.752357	0.000355	−0.003151	0.703663	−0.241550
0.343314	−0.000152	0.002099	0.390159	−0.296938
0.081342	0.000063	−0.000549	0.016378	0.369480
0.041990	−0.000051	0.000445	−0.007958	0.578808
0.020245	0.000016	−0.000135	0.001936	0.232686

	p space	
Exponent	$2p$	$3p$
	−13.629240	−1.340685
6276.263	0.000093	−0.000030
1486.387	0.000819	−0.000268
482.6491	0.004628	−0.001511
184.2216	0.019482	−0.006439
77.70944	0.064185	−0.021514
35.11596	0.162358	−0.056419
16.55729	0.298605	−0.106897
8.005286	0.367466	−0.142558
3.928999	0.233216	−0.057178
1.857387	0.048016	0.233670
0.868676	0.000589	0.478216
0.398356	0.000615	0.369004
0.166299	−0.000157	0.072478

Table XCVIII. Ca ^1S $(22s14p)$ basis set. Energy$(E_H) = -676.758140$

	s space			
Exponent	$1s$	$2s$	$3s$	$4s$
	−149.363700	−16.822730	−2.245364	−0.195524
7503960.	0.000002	−0.000001	0.000000	0.000000
1123486.	0.000017	−0.000005	0.000002	0.000000
255663.5	0.000092	−0.000027	0.000009	−0.000002
72416.06	0.000388	−0.000113	0.000039	−0.000009
23626.04	0.001412	−0.000410	0.000141	−0.000034
8529.986	0.004594	−0.001341	0.000463	−0.000111
3327.341	0.013597	−0.003994	0.001377	−0.000329
1380.354	0.036674	−0.010989	0.003808	−0.000911
602.2149	0.088721	−0.027565	0.009556	−0.002281
273.8874	0.184149	−0.062162	0.021831	−0.005231
128.9451	0.300742	−0.118605	0.042150	−0.010084
62.42299	0.324348	−0.174105	0.064629	−0.015613
30.57437	0.171957	−0.118477	0.045360	−0.010883
13.85522	0.024809	0.194575	−0.082498	0.019958
6.836204	−0.001034	0.546611	−0.323152	0.083487
3.378153	0.001013	0.381263	−0.360633	0.095950
1.491907	−0.000467	0.051878	0.204386	−0.063960
0.721140	0.000187	−0.002050	0.696106	−0.245215
0.334152	−0.000088	0.001688	0.361769	−0.285855
0.082382	0.000034	−0.000397	0.014227	0.370110
0.041655	−0.000026	0.000312	−0.006422	0.591013
0.019973	0.000008	−0.000095	0.001565	0.223172

	p space	
Exponent	$2p$	$3p$
	−13.629250	−1.340696
9339.110	0.000046	−0.000015
2210.971	0.000412	−0.000134
718.1424	0.002364	−0.000773
274.6512	0.010279	−0.003373
116.2980	0.035638	−0.011859
52.83104	0.099242	−0.033758
25.21432	0.211866	−0.074659
12.38631	0.329506	−0.120639
6.219128	0.329291	−0.129243
3.149551	0.157267	0.011841
1.541191	0.023315	0.301773
0.737826	0.000582	0.471964
0.346603	0.000166	0.302321
0.144567	−0.000053	0.047311

Table XCIX. Ca ^1S (22s16p) basis set. Energy(E_H) = −676.758148

		s space		
Exponent	$1s$	$2s$	$3s$	$4s$
	−149.363700	−16.822720	−2.245356	−0.195501
12635220.	0.000001	0.000000	0.000000	0.000000
1890814.	0.000009	−0.000003	0.000001	0.000000
430086.2	0.000048	−0.000014	0.000005	−0.000001
121778.0	0.000203	−0.000059	0.000020	−0.000005
39721.84	0.000739	−0.000215	0.000074	−0.000018
14339.66	0.002412	−0.000702	0.000242	−0.000058
5593.350	0.007193	−0.002105	0.000727	−0.000174
2320.497	0.019760	−0.005837	0.002015	−0.000479
1012.632	0.049698	−0.015053	0.005220	−0.001253
460.9375	0.111807	−0.035471	0.012329	−0.002930
217.3623	0.213498	−0.074794	0.026362	−0.006353
105.6311	0.313150	−0.131912	0.047254	−0.011226
52.60936	0.291087	−0.171216	0.064253	−0.015743
26.50336	0.126521	−0.077892	0.029997	−0.006765
12.54677	0.014706	0.250938	−0.109852	0.025882
6.293949	0.000100	0.544250	−0.338968	0.090026
3.175988	0.000365	0.333151	−0.326991	0.083540
1.456409	−0.000167	0.042212	0.238031	−0.067007
0.703179	0.000019	−0.000266	0.690594	−0.259264
0.326640	−0.000022	0.001035	0.347064	−0.262957
0.067321	0.000003	−0.000084	0.008401	0.657030
0.026578	−0.000001	0.000035	−0.002260	0.519169

	p space	
Exponent	$2p$	$3p$
	−13.629250	−1.340687
412359.1	0.000000	0.000000
13405.82	0.000025	−0.000008
3190.397	0.000217	−0.000071
1038.883	0.001256	−0.000410
398.2929	0.005571	−0.001824
169.2893	0.020020	−0.006614
77.24282	0.059323	−0.019923
37.13156	0.141539	−0.048954
18.47136	0.258291	−0.092211
9.379035	0.340656	−0.128828
4.841955	0.270127	−0.097669
2.491492	0.093387	0.095807
1.253997	0.008927	0.358434
0.617909	0.000655	0.443479
0.297290	−0.000062	0.231700
0.122121	−0.000006	0.027986

Table C. Ca ^1S $(23s15p)$ basis set. Energy$(E_H) = -676.758166$

		s space		
Exponent	$1s$	$2s$	$3s$	$4s$
	−149.363700	−16.822740	−2.245370	−0.195527
12583230.	0.000001	0.000000	0.000000	0.000000
1884722.	0.000009	−0.000003	0.000001	0.000000
429114.2	0.000048	−0.000014	0.000005	−0.000001
121605.6	0.000203	−0.000059	0.000020	−0.000005
39688.79	0.000739	−0.000215	0.000074	−0.000018
14332.73	0.002413	−0.000702	0.000242	−0.000058
5591.768	0.007195	−0.002106	0.000728	−0.000174
2320.138	0.019761	−0.005838	0.002014	−0.000480
1012.582	0.049694	−0.015052	0.005222	−0.001249
460.9642	0.111784	−0.035463	0.012321	−0.002940
217.4029	0.213425	−0.074767	0.026366	−0.006325
105.6677	0.313037	−0.131843	0.047195	−0.011290
52.63832	0.291075	−0.171178	0.064312	−0.015588
26.52267	0.126708	−0.077999	0.029882	−0.007088
12.53896	0.014764	0.251486	−0.109753	0.026634
6.285493	0.000065	0.545107	−0.340707	0.088856
3.166764	0.000380	0.332827	−0.324638	0.085903
1.432853	−0.000179	0.041562	0.248045	−0.076124
0.694955	0.000031	−0.000912	0.687083	−0.247933
0.326331	−0.000029	0.001281	0.337683	−0.276036
0.083411	0.000009	−0.000259	0.012669	0.367636
0.041602	−0.000007	0.000198	−0.005355	0.600511
0.019838	0.000002	−0.000060	0.001298	0.218966

	p space	
Exponent	$2p$	$3p$
	−13.629260	−1.340702
13644.11	0.000024	−0.000008
3229.337	0.000213	−0.000070
1049.011	0.001237	−0.000404
401.5885	0.005503	−0.001802
170.5179	0.019817	−0.006546
77.74394	0.058842	−0.019758
37.35084	0.140708	−0.048652
18.57381	0.257390	−0.091867
9.428930	0.340482	−0.128670
4.867379	0.271355	−0.098500
2.505317	0.094591	0.093685
1.260803	0.009176	0.356963
0.621035	0.000653	0.444366
0.298662	−0.000057	0.233681
0.122830	−0.000007	0.028474

Table CI. Ca ^1S $(23s16p)$ basis set. Energy$(E_H) = -676.758166$

		s space		
Exponent	$1s$	$2s$	$3s$	$4s$
	−149.363700	−16.822740	−2.245371	−0.195527
12937860.	0.000001	0.000000	0.000000	0.000000
1929970.	0.000009	−0.000003	0.000001	0.000000
436987.2	0.000047	−0.000014	0.000005	−0.000001
123202.1	0.000200	−0.000058	0.000020	−0.000005
40067.39	0.000732	−0.000213	0.000073	−0.000018
14439.20	0.002395	−0.000697	0.000240	−0.000057
5626.675	0.007147	−0.002092	0.000723	−0.000173
2332.826	0.019648	−0.005803	0.002002	−0.000478
1017.391	0.049471	−0.014982	0.005197	−0.001244
462.7811	0.111463	−0.035347	0.012281	−0.002930
218.0470	0.213236	−0.074665	0.026326	−0.006316
105.8595	0.313393	−0.131898	0.047216	−0.011293
52.66344	0.291768	−0.171560	0.064441	−0.015622
26.49411	0.126720	−0.077835	0.029844	−0.007071
12.51019	0.014613	0.253181	−0.110628	0.026835
6.267181	0.000091	0.545693	−0.341619	0.089154
3.157351	0.000361	0.330884	−0.323489	0.085516
1.432054	−0.000170	0.041046	0.249843	−0.076469
0.693905	0.000026	−0.000762	0.687104	−0.248498
0.325899	−0.000026	0.001229	0.336627	−0.275149
0.082726	0.000008	−0.000238	0.012540	0.378043
0.041027	−0.000006	0.000182	−0.005362	0.598462
0.019617	0.000002	−0.000056	0.001323	0.210533

	p space	
Exponent	$2p$	$3p$
	−13.629260	−1.340702
406353.1	0.000000	0.000000
13600.72	0.000024	−0.000008
3235.472	0.000212	−0.000069
1053.053	0.001227	−0.000400
403.5688	0.005453	−0.001785
171.4896	0.019627	−0.006482
78.23627	0.058280	−0.019567
37.60652	0.139552	−0.048234
18.70904	0.255927	−0.091319
9.500414	0.339978	−0.128343
4.905567	0.273056	−0.099690
2.526701	0.096427	0.090447
1.271385	0.009574	0.354612
0.626009	0.000647	0.445534
0.300994	−0.000049	0.236840
0.124086	−0.000009	0.029350

Table CII. Sc ^2D $(22s16p8d)$ basis set. Energy(E_H) = −759.735649

	s space			
Exponent	1s	2s	3s	4s
	−165.899900	−19.080580	−2.567285	−0.210094
8414748.	0.000002	−0.000001	0.000000	0.000000
1259880.	0.000017	−0.000005	0.000002	0.000000
286711.1	0.000090	−0.000026	0.000009	−0.000002
81213.35	0.000380	−0.000111	0.000039	−0.000009
26497.17	0.001383	−0.000406	0.000143	−0.000034
9566.893	0.004501	−0.001326	0.000468	−0.000111
3731.903	0.013328	−0.003952	0.001392	−0.000330
1548.215	0.035978	−0.010879	0.003850	−0.000915
675.4697	0.087196	−0.027331	0.009681	−0.002296
307.2292	0.181626	−0.061800	0.022172	−0.005280
144.6618	0.298548	−0.118522	0.043056	−0.010235
70.04387	0.325830	−0.175427	0.066563	−0.015989
34.32379	0.176242	−0.122996	0.048312	−0.011520
15.61457	0.026239	0.189121	−0.082446	0.019812
7.745031	−0.001157	0.546668	−0.332793	0.085708
3.844929	0.001068	0.385422	−0.368897	0.097617
1.720081	−0.000497	0.054192	0.210622	−0.065328
0.832594	0.000197	−0.001710	0.700646	−0.249787
0.385552	−0.000091	0.001645	0.358498	−0.275286
0.096752	0.000034	−0.000358	0.014336	0.349946
0.047792	−0.000026	0.000272	−0.006023	0.599365
0.022364	0.000008	−0.000082	0.001462	0.233295

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−15.668210	−1.574513		−0.343679
22643.53	0.000012	−0.000004	73.56046	0.002248
5358.005	0.000107	−0.000036	21.77393	0.016362
1740.469	0.000624	−0.000209	7.927119	0.063269
666.6273	0.002825	−0.000952	3.186576	0.170406
283.6275	0.010513	−0.003561	1.343727	0.300974
129.7832	0.032828	−0.011265	0.561995	0.373521
62.66790	0.085746	−0.030056	0.227868	0.312533
31.49749	0.179700	−0.065087	0.085264	0.124486
16.23213	0.288666	−0.108264		
8.516991	0.327268	−0.131354		
4.518286	0.209930	−0.054258		
2.366144	0.055555	0.175152		
1.214952	0.003847	0.398072		
0.614271	0.000551	0.398630		
0.300766	−0.000037	0.168584		
0.119984	0.000004	0.015944		

Table CIII. Sc ^2D $(23s16p8d)$ basis set. Energy$(E_H) = -759.735661$

	s space			
Exponent	1s	2s	3s	4s
	−165.899900	−19.080580	−2.567287	−0.210093
13927590.	0.000001	0.000000	0.000000	0.000000
2086917.	0.000009	−0.000003	0.000001	0.000000
475144.6	0.000048	−0.000014	0.000005	−0.000001
134641.3	0.000202	−0.000059	0.000021	−0.000005
43943.38	0.000736	−0.000216	0.000076	−0.000018
15869.97	0.002402	−0.000706	0.000248	−0.000059
6192.056	0.007162	−0.002116	0.000747	−0.000177
2569.439	0.019672	−0.005867	0.002068	−0.000490
1121.476	0.049485	−0.015130	0.005361	−0.001275
510.6065	0.111370	−0.035682	0.012669	−0.003004
240.8825	0.212838	−0.075285	0.027127	−0.006468
117.1282	0.312680	−0.133084	0.048732	−0.011584
58.37339	0.291689	−0.172949	0.066480	−0.016026
29.43808	0.127403	−0.079776	0.031446	−0.007407
14.04546	0.014878	0.250920	−0.112965	0.027256
7.080077	0.000166	0.545802	−0.352538	0.091711
3.585872	0.000310	0.333424	−0.328283	0.086331
1.641716	−0.000149	0.042659	0.259746	−0.079141
0.798895	0.000013	−0.000666	0.689476	−0.252398
0.375394	−0.000021	0.001248	0.331762	−0.264087
0.097842	0.000005	−0.000231	0.012672	0.349300
0.047694	−0.000004	0.000172	−0.004966	0.606780
0.022231	0.000001	−0.000052	0.001198	0.229403

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−15.668210	−1.574514		−0.343680
27510.31	0.000009	−0.000003	73.61358	0.002245
6301.318	0.000082	−0.000028	21.78941	0.016343
2000.000	0.000500	−0.000168	7.932886	0.063208
752.6106	0.002340	−0.000789	3.188861	0.170289
315.7498	0.008973	−0.003036	1.344713	0.300876
142.8340	0.028824	−0.009872	0.562404	0.373532
68.29763	0.077556	−0.027094	0.228019	0.312684
34.05223	0.168132	−0.060668	0.085309	0.124618
17.43511	0.279954	−0.104473		
9.090200	0.332489	−0.132635		
4.798340	0.227875	−0.069194		
2.506610	0.065746	0.152685		
1.283089	0.005075	0.389124		
0.645351	0.000613	0.412632		
0.314768	−0.000035	0.185807		
0.127080	0.000005	0.019021		

Table CIV. Sc ^2D ($21s13p8d$) basis set. Energy(E_H) = -759.735562

	s space			
Exponent	1s	2s	3s	4s
	−165.899800	−19.080560	−2.567270	−0.210084
4789458.	0.000004	−0.000001	0.000001	0.000000
717138.0	0.000035	−0.000010	0.000004	−0.000001
163199.4	0.000182	−0.000053	0.000019	−0.000005
46226.07	0.000768	−0.000225	0.000079	−0.000019
15081.03	0.002789	−0.000820	0.000289	−0.000069
5444.493	0.009027	−0.002666	0.000939	−0.000223
2123.448	0.026350	−0.007901	0.002793	−0.000663
880.5910	0.068882	−0.021260	0.007520	−0.001784
383.7729	0.155633	−0.051441	0.018389	−0.004374
174.1198	0.281710	−0.106415	0.038460	−0.009145
81.55183	0.348180	−0.173529	0.065159	−0.015608
38.76587	0.219361	−0.153272	0.059885	−0.014340
17.22962	0.038915	0.131564	−0.055815	0.013375
8.430348	−0.002085	0.536941	−0.310146	0.079109
4.105819	0.001711	0.434894	−0.402211	0.106795
1.806625	−0.000799	0.067486	0.157394	−0.050448
0.870423	0.000361	−0.002736	0.709174	−0.246184
0.396841	−0.000153	0.002055	0.388296	−0.287153
0.095711	0.000061	−0.000499	0.016580	0.346957
0.048247	−0.000048	0.000392	−0.007527	0.589580
0.022661	0.000015	−0.000118	0.001817	0.242777

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−15.668190	−1.574496		−0.343665
7118.987	0.000090	−0.000030	73.51868	0.002251
1685.915	0.000795	−0.000268	21.76100	0.016378
547.4592	0.004501	−0.001515	7.921755	0.063331
209.0187	0.019016	−0.006480	3.184200	0.170542
88.22638	0.062971	−0.021774	1.342621	0.301100
39.90875	0.160428	−0.057549	0.561524	0.373508
18.85172	0.297534	−0.110199	0.227705	0.312331
9.141763	0.368210	−0.147593	0.085241	0.124351
4.503914	0.234390	−0.057458		
2.143092	0.048826	0.241280		
1.007611	0.000837	0.481849		
0.463154	0.000650	0.361186		
0.193060	−0.000123	0.069486		

Table CV. Sc ^2D ($20s12p9d$) basis set. Energy(E_H) = -759.735416

	s space			
Exponent	1s	2s	3s	4s
	−165.899800	−19.080550	−2.567266	−0.210081
2715278.	0.000009	−0.000003	0.000001	0.000000
406598.4	0.000070	−0.000021	0.000007	−0.000002
92530.04	0.000369	−0.000108	0.000038	−0.000009
26207.92	0.001557	−0.000457	0.000161	−0.000038
8549.429	0.005638	−0.001661	0.000585	−0.000139
3085.975	0.018064	−0.005375	0.001897	−0.000450
1203.172	0.051445	−0.015673	0.005541	−0.001315
498.4869	0.127071	−0.040839	0.014540	−0.003453
216.7360	0.254906	−0.091867	0.033069	−0.007870
97.87476	0.360174	−0.164833	0.061152	−0.014597
45.20433	0.269942	−0.180914	0.070221	−0.016881
20.21187	0.061636	0.051658	−0.021136	0.005117
9.574751	−0.001368	0.504740	−0.270623	0.067919
4.540346	0.002050	0.504601	−0.440683	0.117467
1.995687	−0.000949	0.093904	0.063071	−0.024444
0.942215	0.000429	−0.002926	0.716666	−0.238080
0.417845	−0.000181	0.002437	0.443149	−0.307944
0.095761	0.000082	−0.000677	0.022194	0.309806
0.051351	−0.000068	0.000558	−0.011248	0.576650
0.023878	0.000019	−0.000157	0.002514	0.286671

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−15.668160	−1.574491		−0.343664
4609.885	0.000192	−0.000065	110.2197	0.000981
1092.156	0.001680	−0.000565	32.80041	0.007931
354.3368	0.009276	−0.003141	12.31300	0.033483
134.8076	0.037532	−0.012847	5.063819	0.099652
56.60258	0.114908	−0.040533	2.225547	0.212115
25.33410	0.254424	−0.092868	0.992343	0.315106
11.74033	0.379919	−0.147631	0.436361	0.348109
5.569259	0.309527	−0.112701	0.185705	0.258744
2.594958	0.087011	0.157754	0.073441	0.088899
1.196351	0.002801	0.470453		
0.535059	0.001054	0.429807		
0.220776	−0.000210	0.102956		

Table CVI. Sc ^2D $(21s14p9d)$ basis set. Energy$(E_H) = -759.735629$

	s space			
Exponent	1s	2s	3s	4s
	−165.899900	−19.080590	−2.567299	−0.210099
4788044.	0.000004	−0.000001	0.000001	0.000000
716920.4	0.000035	−0.000010	0.000004	−0.000001
163148.3	0.000182	−0.000053	0.000019	−0.000005
46211.09	0.000768	−0.000225	0.000079	−0.000019
15075.95	0.002790	−0.000821	0.000289	−0.000069
5442.568	0.009031	−0.002668	0.000940	−0.000223
2122.649	0.026362	−0.007905	0.002794	−0.000664
880.2335	0.068916	−0.021270	0.007524	−0.001785
383.6081	0.155699	−0.051465	0.018398	−0.004377
174.0445	0.281783	−0.106453	0.038474	−0.009148
81.51792	0.348162	−0.173555	0.065172	−0.015612
38.75061	0.219242	−0.153197	0.059855	−0.014332
17.22170	0.038862	0.131833	−0.055930	0.013401
8.426406	−0.002084	0.537089	−0.310333	0.079168
4.103964	0.001710	0.434630	−0.402035	0.106742
1.805498	−0.000798	0.067370	0.157931	−0.050588
0.869972	0.000360	−0.002741	0.709157	−0.246286
0.396674	−0.000152	0.002055	0.387923	−0.286999
0.095692	0.000061	−0.000499	0.016505	0.347596
0.048198	−0.000048	0.000392	−0.007473	0.589707
0.022642	0.000015	−0.000118	0.001808	0.242069

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−15.668220	−1.574526		−0.343692
10591.50	0.000045	−0.000015	110.1472	0.000983
2507.305	0.000400	−0.000134	32.77941	0.007941
814.3413	0.002298	−0.000775	12.30502	0.033515
311.4500	0.010023	−0.003391	5.059994	0.099769
131.9186	0.034910	−0.011979	2.223112	0.212402
59.96218	0.097781	−0.034326	0.990815	0.315380
28.64929	0.210340	−0.076566	0.435642	0.347976
14.10260	0.329466	−0.124911	0.185475	0.258308
7.101692	0.330283	−0.133347	0.073382	0.088769
3.608838	0.157994	0.014892		
1.776403	0.023687	0.310369		
0.855101	0.000728	0.472289		
0.402437	0.000210	0.293930		
0.167541	−0.000031	0.045090		

Table CVII. Sc ^2D ($22s14p9d$) basis set. Energy(E_H) = -759.735658

	s space			
Exponent	1s	2s	3s	4s
	−165.899900	−19.080600	−2.567303	−0.210099
8417909.	0.000002	−0.000001	0.000000	0.000000
1260312.	0.000017	−0.000005	0.000002	0.000000
286798.4	0.000090	−0.000026	0.000009	−0.000002
81234.69	0.000380	−0.000111	0.000039	−0.000009
26503.11	0.001383	−0.000406	0.000143	−0.000034
9568.701	0.004500	−0.001326	0.000468	−0.000111
3732.497	0.013326	−0.003951	0.001392	−0.000330
1548.422	0.035974	−0.010877	0.003850	−0.000915
675.5420	0.087189	−0.027328	0.009680	−0.002296
307.2522	0.181623	−0.061799	0.022171	−0.005280
144.6672	0.298558	−0.118524	0.043056	−0.010235
70.04387	0.325846	−0.175438	0.066567	−0.015990
34.32250	0.176242	−0.122988	0.048308	−0.011519
15.61224	0.026233	0.189213	−0.082487	0.019821
7.743722	−0.001159	0.546717	−0.332865	0.085730
3.844260	0.001068	0.385317	−0.368813	0.097592
1.719766	−0.000497	0.054153	0.210771	−0.065366
0.832523	0.000197	−0.001708	0.700541	−0.249776
0.385564	−0.000091	0.001644	0.358477	−0.275246
0.096700	0.000034	−0.000357	0.014364	0.350385
0.047778	−0.000026	0.000272	−0.006050	0.598988
0.022363	0.000008	−0.000082	0.001467	0.233210

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−15.668220	−1.574528		−0.343695
10592.19	0.000045	−0.000015	110.1751	0.000982
2507.533	0.000400	−0.000134	32.78704	0.007937
814.4571	0.002298	−0.000774	12.30757	0.033507
311.5195	0.010019	−0.003390	5.060788	0.099757
131.9617	0.034888	−0.011972	2.223351	0.212395
59.98718	0.097720	−0.034303	0.990910	0.315367
28.66250	0.210249	−0.076532	0.435697	0.347967
14.10851	0.329452	−0.124900	0.185502	0.258335
7.103706	0.330404	−0.133401	0.073391	0.088792
3.609200	0.158072	0.014872		
1.776070	0.023685	0.310551		
0.854760	0.000726	0.472377		
0.402239	0.000210	0.293741		
0.167437	−0.000031	0.045007		

Table CVIII. Sc ^2D $(23s15p10d)$ basis set. Energy$(E_H) = -759.735693$

	s space			
Exponent	1s	2s	3s	4s
	−165.899900	−19.080610	−2.567315	−0.210104
14168980.	0.000001	0.000000	0.000000	0.000000
2121766.	0.000009	−0.000003	0.000001	0.000000
482874.0	0.000047	−0.000014	0.000005	−0.000001
136782.5	0.000198	−0.000058	0.000020	−0.000005
44630.50	0.000722	−0.000212	0.000075	−0.000018
16115.53	0.002357	−0.000692	0.000244	−0.000058
6287.163	0.007029	−0.002077	0.000733	−0.000174
2608.701	0.019318	−0.005759	0.002030	−0.000481
1138.543	0.048639	−0.014864	0.005267	−0.001252
518.3324	0.109685	−0.035089	0.012456	−0.002953
244.4903	0.210395	−0.074242	0.026745	−0.006377
118.8601	0.311217	−0.131714	0.048199	−0.011457
59.23264	0.293889	−0.173037	0.066444	−0.016014
29.86537	0.131356	−0.083374	0.032869	−0.007755
14.13692	0.015864	0.247058	−0.111023	0.026785
7.117886	−0.000064	0.546386	−0.351575	0.091402
3.600310	0.000428	0.336355	−0.330929	0.087079
1.647643	−0.000206	0.043249	0.256624	−0.078251
0.801179	0.000043	−0.000666	0.690358	−0.252266
0.376092	−0.000033	0.001253	0.333580	−0.264854
0.097739	0.000010	−0.000232	0.012781	0.349698
0.047681	−0.000007	0.000172	−0.005037	0.606205
0.022231	0.000002	−0.000052	0.001215	0.229387

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−15.668240	−1.574540		−0.343705
15490.03	0.000023	−0.000008	161.9862	0.000438
3666.169	0.000207	−0.000069	48.32415	0.003800
1190.889	0.001199	−0.000404	18.48303	0.017770
455.9158	0.005347	−0.001805	7.797531	0.056105
193.6296	0.019330	−0.006584	3.502824	0.137420
88.32451	0.057685	−0.019979	1.633143	0.241649
42.46720	0.138886	−0.049576	0.760607	0.316804
21.14808	0.256158	−0.094528	0.349097	0.316569
10.76050	0.341038	−0.133390	0.155021	0.211575
5.570686	0.272620	−0.100875	0.064406	0.063515
2.876952	0.095457	0.099307		
1.454023	0.009455	0.365308		
0.719167	0.000736	0.441478		
0.346155	−0.000009	0.225470		
0.141959	0.000006	0.026910		

Table CIX. Sc ^2D $(23s15p11d)$ basis set. Energy$(E_H) = -759.735695$

	s space			
Exponent	1s	2s	3s	4s
	−165.899900	−19.080610	−2.567317	−0.210105
14228140.	0.000001	0.000000	0.000000	0.000000
2129471.	0.000009	−0.000003	0.000001	0.000000
484447.9	0.000047	−0.000014	0.000005	−0.000001
137186.9	0.000197	−0.000058	0.000020	−0.000005
44749.85	0.000720	−0.000211	0.000074	−0.000018
16154.49	0.002350	−0.000690	0.000243	−0.000058
6300.927	0.007012	−0.002071	0.000731	−0.000174
2613.892	0.019276	−0.005747	0.002026	−0.000480
1140.611	0.048547	−0.014835	0.005256	−0.001250
519.1924	0.109520	−0.035031	0.012435	−0.002948
244.8586	0.210188	−0.074149	0.026710	−0.006368
119.0198	0.311147	−0.131622	0.048162	−0.011448
59.30184	0.294142	−0.173073	0.066452	−0.016015
29.89436	0.131648	−0.083687	0.032991	−0.007785
14.14877	0.015920	0.246585	−0.110777	0.026725
7.123079	−0.000065	0.546401	−0.351420	0.091353
3.602453	0.000429	0.336786	−0.331265	0.087175
1.648130	−0.000206	0.043341	0.256256	−0.078153
0.801428	0.000043	−0.000679	0.690422	−0.252229
0.376178	−0.000033	0.001258	0.333786	−0.264954
0.097759	0.000010	−0.000234	0.012799	0.349354
0.047706	−0.000007	0.000174	−0.005045	0.606175
0.022242	0.000002	−0.000053	0.001217	0.229742

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−15.668240	−1.574542		−0.343707
15494.10	0.000023	−0.000008	232.9690	0.000202
3666.612	0.000207	−0.000069	69.74823	0.001828
1190.924	0.001199	−0.000404	26.92844	0.009375
455.9083	0.005348	−0.001805	11.63805	0.031609
193.6241	0.019331	−0.006584	5.319817	0.083522
88.32299	0.057685	−0.019979	2.550314	0.171141
42.46719	0.138884	−0.049575	1.241813	0.259637
21.14812	0.256161	−0.094529	0.600652	0.309111
10.76030	0.341055	−0.133398	0.286194	0.282576
5.570358	0.272627	−0.100871	0.131955	0.171636
2.876604	0.095440	0.099359	0.057287	0.045303
1.453796	0.009447	0.365373		
0.719029	0.000736	0.441473		
0.346074	−0.000010	0.225390		
0.141907	0.000006	0.026882		

Table CX. Sc ^2D ($21s14p8d$) basis set. Energy(E_H) = -759.735580

	s space			
Exponent	1s	2s	3s	4s
	−165.899800	−19.080570	−2.567277	−0.210089
4787645.	0.000004	−0.000001	0.000001	0.000000
716868.4	0.000035	−0.000010	0.000004	−0.000001
163138.5	0.000182	−0.000053	0.000019	−0.000005
46208.96	0.000768	−0.000225	0.000079	−0.000019
15075.49	0.002790	−0.000821	0.000289	−0.000069
5442.502	0.009031	−0.002668	0.000940	−0.000223
2122.668	0.026361	−0.007904	0.002794	−0.000664
880.2622	0.068912	−0.021269	0.007524	−0.001785
383.6280	0.155688	−0.051461	0.018396	−0.004376
174.0550	0.281772	−0.106447	0.038472	−0.009148
81.52244	0.348168	−0.173554	0.065172	−0.015612
38.75219	0.219260	−0.153205	0.059858	−0.014333
17.22161	0.038867	0.131825	−0.055926	0.013401
8.426540	−0.002087	0.537076	−0.310324	0.079161
4.104056	0.001711	0.434642	−0.402037	0.106745
1.805501	−0.000799	0.067377	0.157906	−0.050590
0.869996	0.000361	−0.002744	0.709141	−0.246251
0.396691	−0.000153	0.002056	0.387946	−0.287029
0.095747	0.000061	−0.000500	0.016511	0.346906
0.048235	−0.000048	0.000392	−0.007468	0.590010
0.022651	0.000015	−0.000118	0.001805	0.242456

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−15.668200	−1.574505		−0.343671
10587.97	0.000045	−0.000015	73.54089	0.002249
2506.580	0.000400	−0.000134	21.76799	0.016369
814.1616	0.002299	−0.000775	7.924830	0.063293
311.4099	0.010024	−0.003392	3.185688	0.170448
131.9160	0.034906	−0.011978	1.343373	0.301000
59.96588	0.097767	−0.034321	0.561870	0.373493
28.65149	0.210332	−0.076562	0.227841	0.312463
14.10289	0.329503	−0.124926	0.085272	0.124477
7.101135	0.330324	−0.133361		
3.608186	0.157962	0.014955		
1.776007	0.023666	0.310471		
0.854884	0.000729	0.472299		
0.402322	0.000209	0.293826		
0.167476	−0.000031	0.045041		

Table CXI. Sc ^2D $(23s16p8d)$ basis set. Energy$(E_H) = -759.735661$

	s space			
Exponent	1s	2s	3s	4s
	−165.899900	−19.080590	−2.567287	−0.210094
14177900.	0.000001	0.000000	0.000000	0.000000
2122423.	0.000009	−0.000003	0.000001	0.000000
482989.8	0.000047	−0.000014	0.000005	−0.000001
136814.9	0.000198	−0.000058	0.000020	−0.000005
44639.80	0.000722	−0.000212	0.000075	−0.000018
16118.06	0.002357	−0.000692	0.000244	−0.000058
6287.794	0.007029	−0.002076	0.000733	−0.000174
2608.845	0.019317	−0.005759	0.002030	−0.000481
1138.574	0.048639	−0.014864	0.005267	−0.001252
518.3339	0.109689	−0.035090	0.012457	−0.002953
244.4816	0.210416	−0.074249	0.026747	−0.006377
118.8482	0.311260	−0.131739	0.048208	−0.011459
59.22179	0.293900	−0.173054	0.066451	−0.016015
29.85755	0.131294	−0.083333	0.032853	−0.007752
14.13699	0.015841	0.247062	−0.111023	0.026785
7.118101	−0.000055	0.546353	−0.351550	0.091391
3.600505	0.000423	0.336386	−0.330939	0.087082
1.647581	−0.000204	0.043260	0.256622	−0.078256
0.801157	0.000042	−0.000671	0.690374	−0.252255
0.376073	−0.000032	0.001255	0.333550	−0.264862
0.097779	0.000010	−0.000233	0.012772	0.349297
0.047699	−0.000007	0.000173	−0.005026	0.606418
0.022237	0.000002	−0.000052	0.001213	0.229586

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−15.668210	−1.574514		−0.343680
22640.97	0.000012	−0.000004	73.56433	0.002248
5357.545	0.000107	−0.000036	21.77497	0.016361
1740.373	0.000624	−0.000209	7.927494	0.063265
666.6163	0.002824	−0.000952	3.186733	0.170398
283.6384	0.010511	−0.003561	1.343799	0.300967
129.7976	0.032819	−0.011262	0.562023	0.373526
62.67956	0.085718	−0.030046	0.227876	0.312544
31.50441	0.179662	−0.065074	0.085266	0.124491
16.23525	0.288656	−0.108257		
8.518324	0.327285	−0.131362		
4.519005	0.209967	−0.054292		
2.366591	0.055583	0.175054		
1.215235	0.003851	0.398039		
0.614348	0.000552	0.398761		
0.300745	−0.000038	0.168602		
0.119948	0.000004	0.015931		

Table CXII. Ti ^3F $(20s12p9d)$ basis set. Energy(E_H) = −848.405659

	s space			
Exponent	1s	2s	3s	4s
	−183.272700	−21.422830	−2.873333	−0.220757
3014643.	0.000009	−0.000003	0.000001	0.000000
451432.9	0.000069	−0.000020	0.000007	−0.000002
102733.8	0.000364	−0.000108	0.000038	−0.000009
29098.17	0.001536	−0.000455	0.000163	−0.000038
9492.330	0.005563	−0.001653	0.000591	−0.000137
3426.346	0.017829	−0.005348	0.001916	−0.000445
1335.896	0.050812	−0.015609	0.005600	−0.001301
553.5026	0.125718	−0.040722	0.014717	−0.003423
240.6925	0.252994	−0.091877	0.033570	−0.007821
108.7293	0.359594	−0.165502	0.062374	−0.014582
50.26457	0.272470	−0.183603	0.072416	−0.017039
22.58004	0.063594	0.047727	−0.019717	0.004651
10.71432	−0.001222	0.505775	−0.278112	0.068492
5.093546	0.002008	0.506638	−0.447909	0.116847
2.244183	−0.000931	0.094617	0.075916	−0.027465
1.059570	0.000414	−0.002760	0.721602	−0.237248
0.468849	−0.000172	0.002400	0.433346	−0.294051
0.106143	0.000074	−0.000625	0.020718	0.314145
0.055262	−0.000060	0.000509	−0.010310	0.575785
0.025465	0.000018	−0.000148	0.002397	0.279404

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−17.791100	−1.795023		−0.440600
5181.157	0.000187	−0.000064	134.3565	0.000919
1227.461	0.001641	−0.000563	40.04189	0.007603
398.2712	0.009083	−0.003143	15.12976	0.033016
151.5867	0.036896	−0.012905	6.276990	0.099467
63.69633	0.113557	−0.040956	2.781410	0.214632
28.54733	0.253188	−0.094609	1.253602	0.319911
13.26129	0.380144	−0.151421	0.557405	0.347625
6.310352	0.310252	−0.114130	0.239759	0.249491
2.951875	0.087678	0.163188	0.095287	0.081345
1.365370	0.003101	0.473366		
0.611415	0.001111	0.424493		
0.252548	−0.000176	0.101422		

Table CXIII. Ti ^3F $(21s13p8d)$ basis set. Energy(E_H) = −848.405786

	s space			
Exponent	1s	2s	3s	4s
	−183.272700	−21.422830	−2.873321	−0.220755
5309148.	0.000004	−0.000001	0.000001	0.000000
794951.6	0.000034	−0.000010	0.000004	−0.000001
180907.6	0.000180	−0.000053	0.000019	−0.000004
51241.93	0.000759	−0.000224	0.000080	−0.000019
16717.45	0.002757	−0.000818	0.000293	−0.000068
6035.266	0.008925	−0.002658	0.000950	−0.000221
2353.857	0.026062	−0.007879	0.002827	−0.000657
976.1465	0.068191	−0.021221	0.007618	−0.001769
425.4356	0.154349	−0.051424	0.018660	−0.004346
193.0468	0.280282	−0.106700	0.039154	−0.009114
90.43937	0.348401	−0.174689	0.066640	−0.015631
43.02071	0.221704	−0.156039	0.062019	−0.014542
19.19056	0.040019	0.129321	−0.055943	0.013123
9.425716	−0.002139	0.538465	−0.319017	0.079806
4.605243	0.001723	0.435707	−0.406593	0.105694
2.037834	−0.000803	0.068117	0.170390	−0.053180
0.980032	0.000356	−0.002435	0.711795	−0.244220
0.445625	−0.000148	0.001987	0.379968	−0.273854
0.106417	0.000057	−0.000456	0.015750	0.342038
0.052571	−0.000044	0.000354	−0.007033	0.589323
0.024357	0.000013	−0.000108	0.001724	0.243560

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−17.791110	−1.795014		−0.440584
7999.805	0.000088	−0.000030	89.56920	0.002124
1894.452	0.000777	−0.000267	26.58436	0.015928
615.1875	0.004404	−0.001515	9.771032	0.062928
234.9274	0.018663	−0.006499	3.961933	0.171507
99.21375	0.062073	−0.021940	1.689269	0.305698
44.91614	0.159074	−0.058362	0.715671	0.375188
21.24972	0.296977	−0.112718	0.293811	0.304401
10.33046	0.368784	−0.151257	0.110831	0.115126
5.104980	0.234859	−0.056822		
2.440690	0.049299	0.247029		
1.151205	0.001078	0.482415		
0.529556	0.000694	0.356299		
0.221190	−0.000098	0.068645		

Table CXIV. Ti ^3F $(22s14p9d)$ basis set. Energy(E_H) = −848.405920

	s space			
Exponent	1s	2s	3s	4s
	−183.272700	−21.422880	−2.873370	−0.220775
9317034.	0.000002	−0.000001	0.000000	0.000000
1394971.	0.000017	−0.000005	0.000002	0.000000
317453.1	0.000089	−0.000026	0.000009	−0.000002
89921.00	0.000376	−0.000111	0.000040	−0.000009
29338.16	0.001369	−0.000405	0.000145	−0.000034
10592.66	0.004456	−0.001324	0.000474	−0.000110
4132.056	0.013198	−0.003946	0.001411	−0.000327
1714.235	0.035642	−0.010867	0.003903	−0.000908
747.9151	0.086466	−0.027327	0.009825	−0.002281
340.1991	0.180445	−0.061897	0.022542	−0.005256
160.2060	0.297547	−0.119055	0.043922	−0.010222
77.58851	0.326512	−0.176914	0.068204	−0.016043
38.04489	0.178213	−0.125472	0.050188	−0.011722
17.35362	0.026886	0.188911	−0.084217	0.019829
8.642062	−0.001236	0.548641	−0.342896	0.086618
4.304404	0.001081	0.384679	−0.370601	0.095989
1.937718	−0.000504	0.054357	0.225170	−0.068275
0.936594	0.000197	−0.001423	0.701817	−0.247408
0.432624	−0.000089	0.001574	0.349998	−0.261869
0.107352	0.000032	−0.000320	0.013628	0.346253
0.052034	−0.000024	0.000242	−0.005660	0.597564
0.024038	0.000007	−0.000074	0.001392	0.234171

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−17.791160	−1.795061		−0.440631
11912.03	0.000044	−0.000015	134.2157	0.000921
2819.947	0.000390	−0.000134	39.99780	0.007619
915.9479	0.002243	−0.000772	15.11145	0.033080
350.3842	0.009804	−0.003389	6.268296	0.099663
148.4825	0.034269	−0.012016	2.776898	0.214957
67.53944	0.096468	−0.034624	1.251422	0.320039
32.30332	0.208964	−0.077837	0.556600	0.347342
15.92786	0.329501	−0.128087	0.239553	0.249133
8.038035	0.331259	−0.136269	0.095230	0.081272
4.093916	0.158617	0.017678		
2.022390	0.024004	0.316271		
0.976102	0.000877	0.470793		
0.459595	0.000257	0.289163		
0.191904	−0.000015	0.044407		

Table CXV. Ti ^3F $(23s15p10d)$ basis set. Energy(E_H) = −848.405967

	s space			
Exponent	1s	2s	3s	4s
	−183.272700	−21.422900	−2.873387	−0.220783
15683520.	0.000001	0.000000	0.000000	0.000000
2348481.	0.000009	−0.000003	0.000001	0.000000
534480.0	0.000046	−0.000014	0.000005	−0.000001
151403.3	0.000196	−0.000058	0.000021	−0.000005
49400.74	0.000715	−0.000212	0.000076	−0.000018
17837.65	0.002334	−0.000691	0.000247	−0.000057
6958.866	0.006963	−0.002074	0.000743	−0.000173
2887.359	0.019140	−0.005754	0.002058	−0.000478
1260.148	0.048220	−0.014859	0.005343	−0.001244
573.6964	0.108872	−0.035118	0.012654	−0.002937
270.6159	0.209275	−0.074451	0.027225	−0.006355
131.5736	0.310617	−0.132480	0.049246	−0.011461
65.58267	0.294970	−0.174788	0.068198	−0.016095
33.08849	0.132992	−0.085441	0.034371	−0.007949
15.69597	0.016217	0.248553	−0.114469	0.027080
7.931523	−0.000123	0.548325	−0.362349	0.092386
4.024297	0.000430	0.334485	−0.329972	0.084961
1.853911	−0.000210	0.043137	0.272045	−0.081299
0.900650	0.000044	−0.000413	0.690227	−0.249415
0.421753	−0.000032	0.001189	0.325053	−0.251500
0.108517	0.000010	−0.000202	0.012127	0.344812
0.052017	−0.000007	0.000150	−0.004714	0.603995
0.023941	0.000002	−0.000046	0.001151	0.231726

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−17.791180	−1.795077		−0.440647
17241.11	0.000023	−0.000008	200.6311	0.000395
4081.984	0.000205	−0.000070	59.81422	0.003509
1326.762	0.001188	−0.000409	22.92199	0.017014
508.3398	0.005298	−0.001827	9.734721	0.055007
216.1104	0.019170	−0.006673	4.397417	0.136887
98.69914	0.057318	−0.020294	2.065602	0.244694
47.52134	0.138421	−0.050552	0.971125	0.320680
23.70680	0.256289	−0.096893	0.449811	0.314893
12.09192	0.341628	−0.137031	0.201390	0.203264
6.276736	0.272023	−0.101180	0.083754	0.058210
3.249948	0.094768	0.106065		
1.647748	0.009477	0.371327		
0.816925	0.000829	0.437092		
0.393455	0.000032	0.219729		
0.161816	0.000015	0.026020		

Table CXVI. Ti ^3F $(23s15p11d)$ basis set. Energy(E_H) = −848.405971

	s space			
Exponent	1s	2s	3s	4s
	−183.272700	−21.422900	−2.873390	−0.220784
15688460.	0.000001	0.000000	0.000000	0.000000
2348898.	0.000009	−0.000003	0.000001	0.000000
534521.8	0.000046	−0.000014	0.000005	−0.000001
151404.7	0.000196	−0.000058	0.000021	−0.000005
49398.75	0.000715	−0.000212	0.000076	−0.000018
17836.39	0.002335	−0.000692	0.000247	−0.000057
6958.296	0.006963	−0.002074	0.000743	−0.000173
2887.139	0.019141	−0.005755	0.002059	−0.000478
1260.075	0.048222	−0.014859	0.005343	−0.001244
573.6763	0.108872	−0.035118	0.012655	−0.002937
270.6123	0.209272	−0.074450	0.027225	−0.006355
131.5738	0.310612	−0.132479	0.049246	−0.011461
65.58311	0.294971	−0.174783	0.068197	−0.016095
33.08875	0.132991	−0.085460	0.034377	−0.007951
15.69888	0.016217	0.248435	−0.114405	0.027065
7.933184	−0.000119	0.548289	−0.362279	0.092365
4.025150	0.000428	0.334620	−0.330076	0.084992
1.854148	−0.000209	0.043175	0.271878	−0.081257
0.900789	0.000044	−0.000418	0.690245	−0.249388
0.421808	−0.000032	0.001192	0.325160	−0.251557
0.108543	0.000009	−0.000203	0.012138	0.344500
0.052043	−0.000007	0.000150	−0.004719	0.603976
0.023952	0.000002	−0.000046	0.001152	0.232049

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−17.791180	−1.795080		−0.440650
17401.20	0.000023	−0.000008	292.1649	0.000177
4118.629	0.000202	−0.000069	87.44018	0.001631
1337.948	0.001172	−0.000403	33.74444	0.008663
512.2883	0.005234	−0.001805	14.64434	0.030265
217.6497	0.018972	−0.006604	6.729229	0.081448
99.34493	0.056833	−0.020118	3.241192	0.170629
47.80830	0.137562	−0.050222	1.589787	0.262900
23.84071	0.255369	−0.096518	0.775083	0.312138
12.15572	0.341531	−0.136904	0.371963	0.280524
6.307978	0.273308	−0.102097	0.172455	0.164685
3.266055	0.095903	0.104089	0.074687	0.041758
1.655382	0.009695	0.370249		
0.820318	0.000829	0.438029		
0.394930	0.000036	0.221294		
0.162526	0.000015	0.026379		

Table CXVII. Ti ^3F $(23s16p8d)$ basis set. Energy(E_H) = −848.405893

	s space			
Exponent	1s	2s	3s	4s
	−183.272700	−21.422860	−2.873339	−0.220764
15697450.	0.000001	0.000000	0.000000	0.000000
2350021.	0.000009	−0.000003	0.000001	0.000000
534780.9	0.000046	−0.000014	0.000005	−0.000001
151482.2	0.000196	−0.000058	0.000021	−0.000005
49424.59	0.000715	−0.000212	0.000076	−0.000018
17845.56	0.002333	−0.000691	0.000247	−0.000057
6961.706	0.006959	−0.002073	0.000742	−0.000173
2888.468	0.019131	−0.005752	0.002057	−0.000477
1260.623	0.048199	−0.014852	0.005341	−0.001243
573.9151	0.108828	−0.035103	0.012649	−0.002936
270.7213	0.209208	−0.074421	0.027214	−0.006352
131.6256	0.310572	−0.132444	0.049232	−0.011458
65.60852	0.295031	−0.174782	0.068194	−0.016093
33.10119	0.133093	−0.085568	0.034422	−0.007962
15.70374	0.016243	0.248244	−0.114308	0.027042
7.935485	−0.000121	0.548284	−0.362198	0.092334
4.026185	0.000430	0.334789	−0.330237	0.085039
1.854634	−0.000210	0.043217	0.271655	−0.081203
0.900960	0.000044	−0.000419	0.690331	−0.249350
0.421851	−0.000032	0.001193	0.325268	−0.251637
0.108618	0.000010	−0.000204	0.012138	0.343749
0.052083	−0.000007	0.000150	−0.004709	0.604359
0.023962	0.000002	−0.000046	0.001149	0.232417

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−17.791130	−1.795032		−0.440598
25537.33	0.000012	−0.000004	89.62535	0.002122
6042.243	0.000104	−0.000035	26.60108	0.015911
1962.653	0.000605	−0.000208	9.777628	0.062868
751.7338	0.002746	−0.000946	3.964659	0.171391
319.8833	0.010246	−0.003546	1.690413	0.305624
146.4300	0.032115	−0.011262	0.716090	0.375253
70.74861	0.084313	−0.030211	0.293922	0.304565
35.59088	0.177948	−0.065938	0.110827	0.115176
18.36893	0.287968	−0.110678		
9.658655	0.328079	−0.134631		
5.136730	0.211293	−0.054477		
2.698872	0.056488	0.179184		
1.389703	0.004134	0.400549		
0.703163	0.000623	0.395313		
0.344123	0.000002	0.166514		
0.137832	0.000009	0.015741		

Table CXVIII. V ^4F $(20s12p9d)$ basis set. Energy(E_H) = −942.883959

	s space			
Exponent	1s	2s	3s	4s
	−201.502700	−23.874570	−3.183112	−0.230545
3321857.	0.000009	−0.000003	0.000001	0.000000
497435.6	0.000069	−0.000020	0.000007	−0.000002
113202.7	0.000361	−0.000108	0.000039	−0.000009
32063.33	0.001522	−0.000454	0.000164	−0.000037
10459.62	0.005512	−0.001650	0.000597	−0.000136
3775.506	0.017669	−0.005340	0.001935	−0.000440
1472.040	0.050383	−0.015593	0.005659	−0.001286
609.9331	0.124809	−0.040723	0.014892	−0.003387
265.2634	0.251726	−0.092084	0.034043	−0.007755
119.8607	0.359226	−0.166364	0.063491	−0.014519
55.44891	0.274165	−0.185806	0.074228	−0.017078
24.98372	0.064862	0.045858	−0.019101	0.004390
11.88056	−0.001164	0.508061	−0.285678	0.068930
5.660311	0.001980	0.506938	−0.452565	0.115396
2.495703	−0.000918	0.094281	0.090265	−0.030795
1.177866	0.000404	−0.002662	0.724845	−0.234891
0.520044	−0.000165	0.002362	0.423304	−0.281164
0.115965	0.000067	−0.000584	0.019347	0.318190
0.058938	−0.000055	0.000472	−0.009539	0.573895
0.026946	0.000016	−0.000140	0.002289	0.273512

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−20.022390	−2.019153		−0.509555
5777.377	0.000184	−0.000064	155.8527	0.000907
1368.674	0.001611	−0.000563	46.49771	0.007591
444.1233	0.008933	−0.003144	17.62999	0.033522
169.0991	0.036409	−0.012956	7.354672	0.101577
71.10191	0.112556	−0.041322	3.274051	0.218831
31.90311	0.252398	−0.096109	1.482482	0.323280
14.85109	0.380464	−0.154605	0.661351	0.345015
7.085227	0.310530	−0.114862	0.284826	0.242966
3.324422	0.087986	0.168234	0.112899	0.077857
1.541164	0.003350	0.475342		
0.690520	0.001163	0.419945		
0.285424	−0.000148	0.100324		

Table CXIX. V ^4F $(20s12p8d)$ basis set. Energy(E_H) = −942.883854

	s space			
Exponent	1s	2s	3s	4s
	−201.502700	−23.874510	−3.183056	−0.230523
3322275.	0.000009	−0.000003	0.000001	0.000000
497498.4	0.000069	−0.000020	0.000007	−0.000002
113216.9	0.000361	−0.000108	0.000039	−0.000009
32067.38	0.001522	−0.000454	0.000164	−0.000037
10460.95	0.005511	−0.001650	0.000597	−0.000136
3775.984	0.017666	−0.005339	0.001935	−0.000440
1472.226	0.050376	−0.015591	0.005658	−0.001286
610.0108	0.124792	−0.040718	0.014890	−0.003387
265.2975	0.251701	−0.092073	0.034039	−0.007754
119.8764	0.359216	−0.166350	0.063485	−0.014517
55.45662	0.274196	−0.185817	0.074233	−0.017079
24.98866	0.064890	0.045770	−0.019064	0.004382
11.88262	−0.001160	0.507975	−0.285597	0.068905
5.661320	0.001979	0.507020	−0.452605	0.115404
2.496419	−0.000917	0.094344	0.090039	−0.030738
1.178113	0.000404	−0.002655	0.724838	−0.234844
0.520125	−0.000165	0.002361	0.423459	−0.281212
0.115997	0.000067	−0.000584	0.019366	0.317674
0.058969	−0.000055	0.000472	−0.009546	0.574161
0.026950	0.000016	−0.000140	0.002288	0.273734

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−20.022340	−2.019100		−0.509496
5780.804	0.000184	−0.000064	104.0005	0.002099
1369.485	0.001610	−0.000562	30.91699	0.016001
444.3868	0.008924	−0.003141	11.42603	0.064086
169.2003	0.036375	−0.012944	4.659214	0.174848
71.14476	0.112469	−0.041288	1.996883	0.310076
31.92258	0.252261	−0.096055	0.849767	0.374546
14.86042	0.380392	−0.154560	0.349538	0.298058
7.089901	0.310687	−0.115003	0.131661	0.110739
3.327095	0.088145	0.167853		
1.542378	0.003374	0.475217		
0.691010	0.001162	0.420251		
0.285616	−0.000147	0.100517		

Table CXX. V ^4F ($21s13p9d$) basis set. Energy(E_H) = -942.884163

	s space			
Exponent	1s	2s	3s	4s
	−201.502800	−23.874600	−3.183138	−0.230557
5845055.	0.000004	−0.000001	0.000001	0.000000
875193.5	0.000034	−0.000010	0.000004	−0.000001
199168.2	0.000178	−0.000053	0.000019	−0.000004
56414.28	0.000752	−0.000224	0.000081	−0.000018
18404.92	0.002735	−0.000817	0.000296	−0.000067
6644.474	0.008853	−0.002657	0.000961	−0.000218
2591.462	0.025859	−0.007876	0.002859	−0.000650
1074.690	0.067705	−0.021228	0.007709	−0.001751
468.4043	0.153453	−0.051504	0.018910	−0.004307
212.5702	0.279298	−0.107111	0.039779	−0.009056
99.60999	0.348556	−0.175880	0.067943	−0.015589
47.41296	0.223325	−0.158222	0.063755	−0.014623
21.20597	0.040766	0.128752	−0.056651	0.013002
10.45031	−0.002195	0.540626	−0.327428	0.080213
5.119088	0.001726	0.435082	−0.408542	0.103824
2.273359	−0.000803	0.068031	0.184075	−0.055917
1.090860	0.000351	−0.002189	0.713008	−0.240882
0.494673	−0.000144	0.001920	0.371492	−0.261700
0.116501	0.000054	−0.000419	0.014897	0.339946
0.056557	−0.000041	0.000323	−0.006609	0.587321
0.025925	0.000013	−0.000099	0.001648	0.243429

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−20.022440	−2.019179		−0.509577
8914.540	0.000086	−0.000030	155.7320	0.000908
2111.022	0.000763	−0.000267	46.46176	0.007602
685.5261	0.004331	−0.001516	17.61565	0.033566
261.8359	0.018406	−0.006520	7.347675	0.101722
110.6275	0.061439	−0.022099	3.270148	0.219097
50.11923	0.158203	−0.059099	1.480464	0.323407
23.74255	0.296862	−0.114928	0.660543	0.344816
11.56717	0.369244	−0.154243	0.284586	0.242671
5.730158	0.234726	−0.055537	0.112832	0.077767
2.749341	0.049445	0.252416		
1.299534	0.001283	0.482451		
0.597918	0.000732	0.351948		
0.250137	−0.000076	0.067938		

Table CXXI. V ^4F ($22s14p10d$) basis set. Energy(E_H) = -942.884269

	s space			
Exponent	1s	2s	3s	4s
	−201.502800	−23.874630	−3.183166	−0.230569
10251780.	0.000002	−0.000001	0.000000	0.000000
1534920.	0.000017	−0.000005	0.000002	0.000000
349300.9	0.000088	−0.000026	0.000010	−0.000002
98942.05	0.000373	−0.000111	0.000040	−0.000009
32281.36	0.001359	−0.000405	0.000146	−0.000033
11655.27	0.004423	−0.001324	0.000480	−0.000109
4546.548	0.013102	−0.003947	0.001427	−0.000324
1886.185	0.035395	−0.010872	0.003950	−0.000899
822.9417	0.085934	−0.027364	0.009953	−0.002260
374.3439	0.179591	−0.062066	0.022871	−0.005215
176.3069	0.296835	−0.119653	0.044684	−0.010171
85.40661	0.327003	−0.178330	0.069623	−0.016018
41.90435	0.179621	−0.127394	0.051710	−0.011818
19.15525	0.027335	0.189794	−0.086268	0.019891
9.571617	−0.001305	0.550758	−0.351951	0.087045
4.780086	0.001088	0.383059	−0.370318	0.093765
2.161860	−0.000507	0.054136	0.238931	−0.070801
1.042711	0.000196	−0.001173	0.701863	−0.243511
0.480282	−0.000087	0.001507	0.342116	−0.250087
0.117638	0.000030	−0.000290	0.012939	0.341983
0.056174	−0.000023	0.000218	−0.005344	0.595131
0.025661	0.000007	−0.000067	0.001330	0.236431

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−20.022470	−2.019207		−0.509603
13273.20	0.000043	−0.000015	229.1891	0.000401
3142.126	0.000383	−0.000134	68.53517	0.003568
1020.588	0.002205	−0.000772	26.35684	0.017456
390.4407	0.009658	−0.003397	11.25785	0.056822
165.5043	0.033864	−0.012080	5.116300	0.140887
75.32006	0.095707	−0.034968	2.415981	0.249806
36.05503	0.208373	−0.079071	1.141345	0.322453
17.80436	0.329917	−0.130893	0.530287	0.310038
9.002929	0.331576	−0.138305	0.237741	0.195781
4.594544	0.158341	0.021090	0.098629	0.054874
2.276760	0.024076	0.321346		
1.101178	0.001016	0.468828		
0.518638	0.000296	0.285137		
0.217134	−0.000001	0.043931		

Table CXXII. V ^4F ($22s15p10d$) basis set. Energy(E_H) = −942.884286

	s space			
Exponent	1s	2s	3s	4s
	−201.502800	−23.874640	−3.183169	−0.230572
10251590.	0.000002	−0.000001	0.000000	0.000000
1534898.	0.000017	−0.000005	0.000002	0.000000
349294.7	0.000088	−0.000026	0.000010	−0.000002
98939.78	0.000373	−0.000111	0.000040	−0.000009
32280.53	0.001359	−0.000405	0.000146	−0.000033
11654.98	0.004423	−0.001324	0.000480	−0.000109
4546.443	0.013102	−0.003947	0.001427	−0.000324
1886.149	0.035395	−0.010873	0.003950	−0.000899
822.9329	0.085934	−0.027364	0.009953	−0.002260
374.3444	0.179588	−0.062065	0.022870	−0.005215
176.3089	0.296830	−0.119651	0.044683	−0.010171
85.40822	0.327001	−0.178328	0.069622	−0.016018
41.90539	0.179627	−0.127399	0.051712	−0.011819
19.15599	0.027338	0.189766	−0.086254	0.019888
9.572134	−0.001305	0.550735	−0.351924	0.087039
4.780389	0.001088	0.383097	−0.370345	0.093773
2.161934	−0.000507	0.054152	0.238888	−0.070790
1.042727	0.000196	−0.001176	0.701903	−0.243524
0.480266	−0.000087	0.001508	0.342111	−0.250096
0.117660	0.000030	−0.000290	0.012922	0.341867
0.056179	−0.000023	0.000218	−0.005329	0.595244
0.025661	0.000007	−0.000067	0.001327	0.236446

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−20.022470	−2.019211		−0.509606
19457.24	0.000022	−0.000008	229.0224	0.000402
4604.858	0.000197	−0.000069	68.48511	0.003573
1495.797	0.001145	−0.000400	26.33704	0.017478
572.7173	0.005123	−0.001797	11.24863	0.056891
243.3576	0.018624	−0.006595	5.111769	0.141028
111.1192	0.056008	−0.020173	2.413808	0.249914
53.50554	0.136283	−0.050654	1.140440	0.322410
26.70955	0.254583	−0.098083	0.529988	0.309874
13.64149	0.341945	−0.139768	0.237668	0.195668
7.092912	0.274050	−0.103061	0.098605	0.054852
3.680287	0.096487	0.107672		
1.869437	0.009972	0.373366		
0.927539	0.000919	0.435129		
0.446537	0.000077	0.218977		
0.184477	0.000023	0.026283		

Table CXXIII. V ^4F $(22s15p8d)$ basis set. Energy$(E_H) = -942.884153$

	s space			
Exponent	1s	2s	3s	4s
	0.000000	0.000000	0.000000	0.000000
10252880.	0.000002	−0.000001	0.000000	0.000000
1535082.	0.000017	−0.000005	0.000002	0.000000
349338.9	0.000088	−0.000026	0.000010	−0.000002
98953.26	0.000373	−0.000111	0.000040	−0.000009
32285.08	0.001359	−0.000405	0.000146	−0.000033
11656.63	0.004422	−0.001324	0.000480	−0.000109
4547.076	0.013100	−0.003946	0.001427	−0.000324
1886.406	0.035390	−0.010871	0.003950	−0.000899
823.0437	0.085921	−0.027360	0.009951	−0.002259
374.3941	0.179568	−0.062057	0.022867	−0.005214
176.3318	0.296811	−0.119639	0.044679	−0.010169
85.41895	0.327013	−0.178322	0.069619	−0.016016
41.91039	0.179663	−0.127428	0.051724	−0.011821
19.15831	0.027351	0.189688	−0.086217	0.019879
9.573348	−0.001306	0.550704	−0.351871	0.087016
4.781033	0.001089	0.383169	−0.370408	0.093790
2.162375	−0.000508	0.054184	0.238695	−0.070744
1.042937	0.000196	−0.001176	0.701912	−0.243459
0.480349	−0.000087	0.001509	0.342258	−0.250166
0.117730	0.000030	−0.000290	0.012938	0.341050
0.056232	−0.000023	0.000218	−0.005330	0.595547
0.025675	0.000007	−0.000067	0.001324	0.236934

	p space		d space	
Exponent	2p	3p	Exponent	3d
	0.000000	0.000000		0.000000
19428.53	0.000022	−0.000008	104.0677	0.002096
4598.102	0.000198	−0.000069	30.93725	0.015983
1493.614	0.001148	−0.000402	11.43435	0.064016
571.8846	0.005135	−0.001801	4.663133	0.174674
243.0049	0.018666	−0.006610	1.998890	0.309892
110.9586	0.056123	−0.020215	0.850682	0.374573
53.42832	0.136511	−0.050742	0.349864	0.298329
26.67006	0.254886	−0.098209	0.131707	0.110900
13.62023	0.342089	−0.139850		
7.080756	0.273726	−0.102786		
3.672784	0.096071	0.108590		
1.864867	0.009867	0.374228		
0.925040	0.000917	0.434783		
0.445299	0.000074	0.217908		
0.183852	0.000023	0.026004		

Table CXXIV. V ^4F ($23s15p11d$) basis set. Energy(E_H) = −942.884309

	s space			
Exponent	1s	2s	3s	4s
	−201.502800	−23.874640	−3.183177	−0.230574
17242380.	0.000001	0.000000	0.000000	0.000000
2581538.	0.000009	−0.000003	0.000001	0.000000
587483.2	0.000046	−0.000014	0.000005	−0.000001
166412.7	0.000195	−0.000058	0.000021	−0.000005
54297.20	0.000711	−0.000212	0.000077	−0.000017
19605.57	0.002320	−0.000692	0.000250	−0.000057
7648.605	0.006920	−0.002077	0.000752	−0.000171
3173.588	0.019027	−0.005763	0.002086	−0.000473
1385.106	0.047952	−0.014888	0.005415	−0.001233
630.6174	0.108351	−0.035216	0.012840	−0.002915
297.4967	0.208559	−0.074767	0.027665	−0.006316
144.6682	0.310230	−0.133323	0.050180	−0.011423
72.13115	0.295650	−0.176374	0.069701	−0.016089
36.41856	0.134015	−0.086822	0.035498	−0.008037
17.31292	0.016424	0.250907	−0.118019	0.027350
8.775325	−0.000166	0.550176	−0.371795	0.092806
4.463181	0.000426	0.331991	−0.327250	0.082328
2.065646	−0.000210	0.042741	0.286425	−0.083782
1.001966	0.000044	−0.000207	0.689039	−0.245136
0.467938	−0.000031	0.001132	0.317152	−0.239762
0.118803	0.000009	−0.000179	0.011493	0.341149
0.056122	−0.000007	0.000132	−0.004450	0.601011
0.025550	0.000002	−0.000041	0.001100	0.233779

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−20.022480	−2.019217		−0.509613
19450.88	0.000022	−0.000008	332.1785	0.000181
4603.366	0.000197	−0.000069	99.66854	0.001670
1495.313	0.001146	−0.000401	38.56667	0.008920
572.5294	0.005126	−0.001798	16.80678	0.031423
243.2758	0.018634	−0.006598	7.766794	0.084615
111.0804	0.056037	−0.020184	3.760123	0.175919
53.48658	0.136337	−0.050675	1.853090	0.267819
26.70074	0.254631	−0.098103	0.907260	0.311920
13.63759	0.341942	−0.139771	0.436592	0.273978
7.091043	0.273985	−0.103013	0.202699	0.157012
3.679236	0.096427	0.107802	0.087554	0.038889
1.868736	0.009957	0.373527		
0.927105	0.000918	0.435095		
0.446316	0.000076	0.218780		
0.184372	0.000023	0.026234		

Table CXXV. V ^4F $(23s16p8d)$ basis set. Energy$(E_H) = -942.884174$

	s space			
Exponent	1s	2s	3s	4s
	−201.502800	−23.874570	−3.183099	−0.230545
17228890.	0.000001	0.000000	0.000000	0.000000
2579749.	0.000009	−0.000003	0.000001	0.000000
587081.5	0.000046	−0.000014	0.000005	−0.000001
166293.3	0.000195	−0.000058	0.000021	−0.000005
54256.91	0.000711	−0.000212	0.000077	−0.000017
19591.10	0.002322	−0.000693	0.000250	−0.000057
7643.165	0.006926	−0.002079	0.000753	−0.000171
3171.454	0.019041	−0.005768	0.002087	−0.000474
1384.235	0.047984	−0.014898	0.005419	−0.001234
630.2472	0.108412	−0.035237	0.012848	−0.002916
297.3331	0.208642	−0.074803	0.027679	−0.006318
144.5935	0.310272	−0.133366	0.050197	−0.011426
72.09616	0.295566	−0.176369	0.069701	−0.016088
36.40226	0.133887	−0.086692	0.035446	−0.008025
17.30742	0.016394	0.251104	−0.118125	0.027374
8.772773	−0.000162	0.550171	−0.371862	0.092819
4.462089	0.000424	0.331820	−0.327091	0.082282
2.065224	−0.000209	0.042703	0.286626	−0.083838
1.001765	0.000044	−0.000206	0.689001	−0.245126
0.467857	−0.000031	0.001132	0.317018	−0.239711
0.118842	0.000009	−0.000179	0.011476	0.340827
0.056126	−0.000007	0.000132	−0.004434	0.601467
0.025542	0.000002	−0.000041	0.001095	0.233652

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−20.022410	−2.019145		−0.509534
28563.32	0.000011	−0.000004	104.0286	0.002097
6757.191	0.000101	−0.000035	30.92688	0.015992
2194.652	0.000591	−0.000206	11.43072	0.064043
840.5257	0.002685	−0.000941	4.661763	0.174721
357.6666	0.010042	−0.003536	1.998320	0.309929
163.7534	0.031586	−0.011268	0.850440	0.374570
79.14466	0.083296	−0.030376	0.349764	0.298272
39.83858	0.176820	−0.066729	0.131671	0.110842
20.58536	0.287747	−0.112810		
10.84307	0.328691	−0.137271		
5.777969	0.211866	−0.053933		
3.043170	0.056932	0.183279		
1.570239	0.004349	0.402267		
0.794975	0.000689	0.391973		
0.388980	0.000036	0.164844		
0.156464	0.000014	0.015638		

Table CXXVI. Cr ^7S $(20s12p9d)$ basis set. Energy(E_H) = −1043.355952 .

	s space			
Exponent	1s	2s	3s	4s
	−220.386200	−26.209470	−3.284998	−0.221964
6177194.	0.000005	−0.000001	0.000001	0.000000
924929.5	0.000035	−0.000011	0.000004	−0.000001
210486.5	0.000185	−0.000055	0.000020	−0.000004
59620.05	0.000782	−0.000234	0.000085	−0.000018
19450.76	0.002840	−0.000855	0.000310	−0.000066
7022.056	0.009191	−0.002778	0.001005	−0.000212
2738.763	0.026820	−0.008233	0.002992	−0.000634
1135.814	0.070067	−0.022154	0.008053	−0.001696
495.0923	0.158023	−0.053644	0.019739	−0.004195
224.7487	0.284680	−0.110845	0.041241	−0.008690
105.3836	0.347841	−0.179811	0.069816	−0.014999
50.19359	0.214697	−0.153263	0.061958	−0.012989
22.24957	0.036390	0.157050	−0.070324	0.014496
10.98265	−0.002337	0.557973	−0.351971	0.081605
5.383665	0.001573	0.406444	−0.383202	0.088512
2.343685	−0.000699	0.054827	0.266921	−0.069750
1.105202	0.000279	−0.001805	0.706754	−0.242433
0.487848	−0.000099	0.001427	0.313804	−0.193710
0.089599	0.000019	−0.000035	0.006973	0.600049
0.033423	−0.000008	0.000166	−0.002071	0.543141

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−22.139670	−2.050770		−0.373458
6268.921	0.000187	−0.000066	150.8341	0.001167
1485.118	0.001644	−0.000576	44.99723	0.009543
481.9146	0.009120	−0.003221	16.96088	0.040911
183.5142	0.037197	−0.013277	7.040154	0.119653
77.19005	0.114922	−0.042379	3.103878	0.238482
34.65178	0.256940	−0.098334	1.375896	0.324558
16.14846	0.383333	−0.156988	0.592282	0.327742
7.710939	0.304791	−0.108586	0.242138	0.240651
3.607154	0.082332	0.184802	0.091284	0.090699
1.667362	0.002897	0.476043		
0.739088	0.001240	0.406661		
0.301326	−0.000071	0.101867		

Table CXXVII. Cr ^7S $(22s14p10d)$ basis set. Energy(E_H) = −1043.356280

	s space			
Exponent	1s	2s	3s	4s
	−220.386400	−26.209590	−3.285118	−0.222031
11016640.	0.000002	−0.000001	0.000000	0.000000
1649423.	0.000017	−0.000005	0.000002	0.000000
375358.9	0.000090	−0.000027	0.000010	−0.000002
106323.6	0.000380	−0.000114	0.000041	−0.000009
34689.76	0.001383	−0.000415	0.000150	−0.000032
12524.83	0.004499	−0.001357	0.000492	−0.000104
4885.752	0.013324	−0.004042	0.001463	−0.000309
2026.918	0.035977	−0.011134	0.004051	−0.000857
884.3645	0.087249	−0.028006	0.010197	−0.002155
402.3170	0.181881	−0.063469	0.023431	−0.004966
189.5271	0.298992	−0.122006	0.045648	−0.009678
91.86095	0.325747	−0.180527	0.070755	−0.015116
45.12476	0.175548	−0.124527	0.050696	−0.010834
20.62512	0.025825	0.204244	−0.094038	0.020344
10.31973	−0.001276	0.557777	−0.365233	0.083643
5.157723	0.000995	0.368776	−0.353168	0.084197
2.312628	−0.000459	0.048584	0.281753	−0.079474
1.103079	0.000171	−0.001050	0.690080	−0.225912
0.498042	−0.000075	0.001357	0.317511	−0.210274
0.118247	0.000027	−0.000213	0.012732	0.278074
0.057356	−0.000020	0.000319	−0.005470	0.597446
0.025760	0.000006	−0.000010	0.001195	0.276769

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−22.139810	−2.050891		−0.373568
14454.20	0.000044	−0.000015	220.4620	0.000525
3421.676	0.000388	−0.000136	65.91007	0.004596
1111.387	0.002237	−0.000785	25.26682	0.021775
425.1918	0.009804	−0.003459	10.72188	0.069128
180.2623	0.034409	−0.012313	4.849489	0.161925
82.06117	0.097280	−0.035687	2.258944	0.264193
39.29726	0.211584	−0.080676	1.042159	0.315970
19.41959	0.333275	−0.133168	0.466342	0.292907
9.828899	0.329359	−0.136726	0.199221	0.197790
5.016810	0.152372	0.031703	0.079226	0.065424
2.487091	0.022223	0.329312		
1.198780	0.001187	0.459384		
0.558695	0.000335	0.280771		
0.234400	0.000060	0.048216		

Table CXXVIII. Cr ^7S $(23s15p11d)$ basis set. Energy(E_H) = −1043.356338

	s space			
Exponent	1s	2s	3s	4s
	−220.386400	−26.209620	−3.285144	−0.222044
18273400.	0.000001	0.000000	0.000000	0.000000
2736169.	0.000009	−0.000003	0.000001	0.000000
622721.5	0.000048	−0.000014	0.000005	−0.000001
176403.1	0.000202	−0.000061	0.000022	−0.000005
57557.12	0.000735	−0.000221	0.000080	−0.000017
20782.05	0.002401	−0.000721	0.000261	−0.000055
8107.214	0.007159	−0.002164	0.000785	−0.000166
3363.697	0.019672	−0.006003	0.002175	−0.000459
1467.989	0.049512	−0.015498	0.005645	−0.001195
668.3000	0.111551	−0.036610	0.013367	−0.002825
315.2450	0.213424	−0.077500	0.028739	−0.006098
153.2895	0.313497	−0.137255	0.051811	−0.010986
76.43130	0.291404	−0.178101	0.070749	−0.015165
38.62445	0.126181	−0.078107	0.032029	−0.006790
18.45229	0.014358	0.272852	−0.130774	0.028387
9.368285	−0.000010	0.553995	−0.386060	0.089362
4.770990	0.000291	0.311636	−0.300915	0.071326
2.195598	−0.000152	0.036819	0.333532	−0.093097
1.052208	0.000018	0.000005	0.673883	−0.226947
0.481567	−0.000019	0.000954	0.289628	−0.198961
0.117447	0.000005	−0.000086	0.010770	0.294502
0.055904	−0.000004	0.000224	−0.004402	0.599986
0.025233	0.000001	0.000015	0.000959	0.260034

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−22.139840	−2.050916		−0.373591
21337.79	0.000022	−0.000008	317.6249	0.000241
5049.498	0.000197	−0.000069	95.21465	0.002199
1640.131	0.001148	−0.000402	36.79532	0.011420
627.9602	0.005140	−0.001808	15.93886	0.039087
266.8501	0.018713	−0.006646	7.330955	0.101821
121.8754	0.056373	−0.020371	3.522099	0.196589
58.70856	0.137361	−0.051260	1.707372	0.275648
29.32725	0.256696	−0.099415	0.814777	0.299549
14.99649	0.343234	−0.141093	0.377532	0.258937
7.805030	0.271475	−0.099847	0.167818	0.161866
4.049328	0.093454	0.116054	0.069956	0.047283
2.056389	0.009479	0.374870		
1.015724	0.001063	0.424931		
0.484463	0.000135	0.220809		
0.203572	0.000068	0.030793		

Table CXXIX. Cr ^5D ($20s12p9d$) basis set. Energy(E_H) = -1043.309392 .

	s space			
Exponent	1s	2s	3s	4s
	−220.592100	−26.439040	−3.499015	−0.239702
3638305.	0.000009	−0.000003	0.000001	0.000000
544822.5	0.000068	−0.000020	0.000007	−0.000002
123986.8	0.000359	−0.000108	0.000039	−0.000009
35117.88	0.001512	−0.000454	0.000166	−0.000037
11456.10	0.005476	−0.001651	0.000602	−0.000134
4135.206	0.017557	−0.005342	0.001954	−0.000434
1612.295	0.050084	−0.015606	0.005716	−0.001270
668.0686	0.124182	−0.040792	0.015060	−0.003350
290.5773	0.250869	−0.092401	0.034485	−0.007681
131.3286	0.359000	−0.167315	0.064515	−0.014430
60.78704	0.275336	−0.187672	0.075767	−0.017045
27.44308	0.065683	0.045233	−0.018997	0.004259
13.08202	−0.001163	0.510933	−0.293025	0.069243
6.244786	0.001961	0.506228	−0.455426	0.113485
2.753437	−0.000908	0.093426	0.104725	−0.034015
1.298441	0.000397	−0.002589	0.726895	−0.231737
0.572030	−0.000160	0.002321	0.413654	−0.269376
0.125502	0.000063	−0.000549	0.018118	0.321611
0.062470	−0.000050	0.000442	−0.008891	0.571851
0.028354	0.000015	−0.000133	0.002192	0.268596

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−22.365160	−2.248740		−0.569087
6399.333	0.000181	−0.000064	177.0182	0.000907
1515.982	0.001587	−0.000562	52.85958	0.007660
491.9534	0.008813	−0.003146	20.09064	0.034236
187.3677	0.036027	−0.013003	8.416376	0.104090
78.82903	0.111802	−0.041650	3.759310	0.223015
35.40597	0.251912	−0.097437	1.706759	0.325809
16.51195	0.380832	−0.157341	0.762211	0.342106
7.895010	0.310519	−0.115133	0.327886	0.237812
3.713305	0.088063	0.172910	0.129421	0.075692
1.724220	0.003558	0.476759		
0.772673	0.001210	0.415942		
0.319507	−0.000123	0.099473		

Table CXXX. Cr ^5D $(21s13p10d)$ basis set. Energy$(E_H) = -1043.309655$

	s space			
Exponent	1s	2s	3s	4s
	−220.592200	−26.439100	−3.499065	−0.239723
6400283.	0.000004	−0.000001	0.000001	0.000000
958328.4	0.000034	−0.000010	0.000004	−0.000001
218087.3	0.000177	−0.000053	0.000019	−0.000004
61773.12	0.000748	−0.000224	0.000082	−0.000018
20153.24	0.002718	−0.000818	0.000299	−0.000066
7275.660	0.008799	−0.002659	0.000970	−0.000215
2837.644	0.025706	−0.007883	0.002888	−0.000642
1176.795	0.067340	−0.021258	0.007792	−0.001731
512.9287	0.152786	−0.051629	0.019137	−0.004263
232.8031	0.278574	−0.107571	0.040339	−0.008980
109.1163	0.348679	−0.177047	0.069100	−0.015505
51.96763	0.224523	−0.160031	0.065219	−0.014632
23.29072	0.041297	0.129088	−0.057669	0.012953
11.51150	−0.002251	0.542989	−0.335204	0.080382
5.651093	0.001726	0.433753	−0.408972	0.101580
2.515856	−0.000799	0.067609	0.197222	−0.058349
1.204328	0.000346	−0.001982	0.713335	−0.236849
0.544628	−0.000139	0.001856	0.363537	−0.250742
0.126307	0.000050	−0.000388	0.014108	0.338441
0.060382	−0.000039	0.000298	−0.006249	0.585019
0.027417	0.000012	−0.000093	0.001582	0.243270

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−22.365230	−2.248790		−0.569134
9869.129	0.000085	−0.000030	260.1153	0.000401
2337.028	0.000752	−0.000267	77.85239	0.003590
758.9317	0.004274	−0.001517	29.98075	0.017757
289.9202	0.018201	−0.006539	12.84703	0.058293
122.5430	0.060946	−0.022241	5.859939	0.144212
55.55327	0.157577	−0.059748	2.775408	0.253733
26.34725	0.296942	−0.116871	1.314136	0.323321
12.86013	0.369624	−0.156726	0.610724	0.306190
6.383714	0.234353	−0.054017	0.273318	0.191151
3.071679	0.049463	0.257149	0.112834	0.053215
1.454135	0.001465	0.482125		
0.669020	0.000767	0.348256		
0.280229	−0.000057	0.067459		

Table CXXXI. Cr ^5D ($22s14p10d$) basis set. Energy(E_H) = −1043.309739

	s space			
Exponent	1s	2s	3s	4s
	−220.592200	−26.439120	−3.499076	−0.239729
11217010.	0.000002	−0.000001	0.000000	0.000000
1679421.	0.000017	−0.000005	0.000002	0.000000
382184.7	0.000088	−0.000026	0.000010	−0.000002
108256.7	0.000371	−0.000111	0.000041	−0.000009
35320.47	0.001352	−0.000406	0.000148	−0.000033
12752.58	0.004400	−0.001326	0.000485	−0.000108
4974.607	0.013034	−0.003953	0.001443	−0.000320
2063.781	0.035222	−0.010893	0.003995	−0.000889
900.4425	0.085565	−0.027433	0.010072	−0.002236
409.6205	0.179008	−0.062294	0.023174	−0.005167
192.9456	0.296362	−0.120307	0.045376	−0.010101
93.48965	0.327343	−0.179680	0.070880	−0.015948
45.89864	0.180561	−0.128861	0.052945	−0.011839
21.02088	0.027619	0.191486	−0.088544	0.019990
10.53387	−0.001359	0.552949	−0.360213	0.087193
5.271854	0.001086	0.380836	−0.368624	0.091205
2.391915	−0.000506	0.053626	0.252169	−0.072995
1.151082	0.000193	−0.000969	0.701126	−0.239045
0.528714	−0.000084	0.001445	0.334563	−0.239414
0.127553	0.000029	−0.000264	0.012270	0.339606
0.060063	−0.000021	0.000198	−0.005066	0.592439
0.027174	0.000007	−0.000061	0.001278	0.237353

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−22.365250	−2.248801		−0.569143
14703.54	0.000042	−0.000015	260.0907	0.000401
3480.679	0.000377	−0.000133	77.84382	0.003590
1130.558	0.002172	−0.000771	29.97719	0.017761
432.5452	0.009530	−0.003400	12.84524	0.058308
183.4015	0.033509	−0.012124	5.858355	0.144294
83.50403	0.095042	−0.035237	2.773885	0.253912
40.00274	0.207873	−0.080100	1.313081	0.323413
19.77983	0.330311	−0.133287	0.610231	0.306046
10.01878	0.331831	−0.139916	0.273166	0.190967
5.121161	0.158086	0.024189	0.112792	0.053175
2.543573	0.024144	0.325478		
1.231969	0.001140	0.466909		
0.580217	0.000332	0.281949		
0.243474	0.000011	0.043672		

Table CXXXII. Cr ^5D $(22s15p11d)$ basis set. Energy(E_H) = −1043.309769

	s space			
Exponent	1s	2s	3s	4s
	−220.592200	−26.439130	−3.499087	−0.239735
11216690.	0.000002	−0.000001	0.000000	0.000000
1679406.	0.000017	−0.000005	0.000002	0.000000
382185.0	0.000088	−0.000026	0.000010	−0.000002
108257.6	0.000371	−0.000111	0.000041	−0.000009
35320.98	0.001352	−0.000406	0.000148	−0.000033
12752.84	0.004400	−0.001326	0.000485	−0.000108
4974.728	0.013034	−0.003953	0.001443	−0.000320
2063.839	0.035221	−0.010893	0.003995	−0.000889
900.4735	0.085560	−0.027432	0.010072	−0.002236
409.6386	0.178998	−0.062291	0.023173	−0.005167
192.9559	0.296351	−0.120300	0.045373	−0.010100
93.49520	0.327345	−0.179675	0.070878	−0.015947
45.90164	0.180578	−0.128877	0.052952	−0.011840
21.02298	0.027626	0.191420	−0.088512	0.019983
10.53505	−0.001358	0.552918	−0.360165	0.087181
5.272480	0.001086	0.380905	−0.368687	0.091224
2.392251	−0.000506	0.053653	0.252042	−0.072962
1.151202	0.000193	−0.000970	0.701181	−0.239051
0.528736	−0.000084	0.001446	0.334619	−0.239448
0.127583	0.000029	−0.000264	0.012262	0.339398
0.060081	−0.000021	0.000198	−0.005055	0.592479
0.027180	0.000007	−0.000062	0.001275	0.237528

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−22.365260	−2.248812		−0.569153
21561.59	0.000022	−0.000008	376.6224	0.000181
5102.908	0.000194	−0.000069	113.0992	0.001679
1657.598	0.001127	−0.000400	43.80055	0.009042
634.6951	0.005047	−0.001796	19.12770	0.032194
269.7395	0.018392	−0.006605	8.868850	0.086972
123.2103	0.055480	−0.020271	4.305656	0.179921
59.36112	0.135537	−0.051131	2.126670	0.271316
29.66152	0.254339	−0.099572	1.042614	0.311334
15.17270	0.342405	−0.142257	0.501549	0.269356
7.902384	0.274134	−0.103326	0.232433	0.152588
4.106918	0.096471	0.111704	0.099885	0.037546
2.089481	0.010116	0.376311		
1.037528	0.001000	0.432165		
0.499404	0.000111	0.216473		
0.206973	0.000030	0.026113		

Table CXXXIII. Cr ^5D $(22s15p8d)$ basis set. Energy(E_H) = −1043.309557

	s space			
Exponent	1s	2s	3s	4s
	−220.592100	−26.439030	−3.498977	−0.239694
11218910.	0.000002	−0.000001	0.000000	0.000000
1679708.	0.000017	−0.000005	0.000002	0.000000
382248.0	0.000088	−0.000026	0.000010	−0.000002
108274.2	0.000371	−0.000111	0.000041	−0.000009
35326.04	0.001352	−0.000406	0.000148	−0.000033
12754.54	0.004399	−0.001326	0.000485	−0.000108
4975.342	0.013032	−0.003953	0.001443	−0.000320
2064.075	0.035217	−0.010891	0.003994	−0.000888
900.5687	0.085552	−0.027429	0.010071	−0.002236
409.6786	0.178985	−0.062285	0.023170	−0.005166
192.9732	0.296340	−0.120293	0.045371	−0.010099
93.50289	0.327355	−0.179672	0.070876	−0.015945
45.90505	0.180601	−0.128897	0.052960	−0.011842
21.02449	0.027634	0.191376	−0.088489	0.019978
10.53579	−0.001359	0.552903	−0.360137	0.087163
5.272881	0.001087	0.380945	−0.368716	0.091230
2.392473	−0.000506	0.053672	0.251932	−0.072938
1.151344	0.000193	−0.000972	0.701161	−0.238980
0.528804	−0.000084	0.001447	0.334719	−0.239493
0.127665	0.000029	−0.000264	0.012276	0.338508
0.060143	−0.000021	0.000198	−0.005055	0.592828
0.027194	0.000007	−0.000062	0.001272	0.238042

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−22.365160	−2.248709		−0.569041
21559.55	0.000022	−0.000008	118.3451	0.002097
5102.294	0.000194	−0.000069	35.22408	0.016184
1657.365	0.001127	−0.000400	13.07042	0.065474
634.5944	0.005049	−0.001796	5.354081	0.178270
269.6918	0.018397	−0.006607	2.302873	0.313586
123.1862	0.055497	−0.020278	0.982113	0.373302
59.34843	0.135575	−0.051145	0.403646	0.293129
29.65410	0.254407	−0.099601	0.151391	0.108195
15.16782	0.342472	−0.142285		
7.898846	0.274095	−0.103278		
4.104122	0.096357	0.112077		
2.086998	0.010076	0.376903		
1.035840	0.000996	0.432101		
0.498469	0.000110	0.215802		
0.206491	0.000030	0.025920		

Table CXXXIV. Cr ^5D ($23s15p11d$) basis set. Energy(E_H) = -1043.309786

	s space			
Exponent	1s	2s	3s	4s
	−220.592200	−26.439130	−3.499089	−0.239735
18860890.	0.000001	0.000000	0.000000	0.000000
2823544.	0.000009	−0.000003	0.000001	0.000000
642504.9	0.000046	−0.000014	0.000005	−0.000001
181987.7	0.000194	−0.000058	0.000021	−0.000005
59376.44	0.000707	−0.000212	0.000078	−0.000017
21438.86	0.002309	−0.000694	0.000253	−0.000056
8363.589	0.006890	−0.002082	0.000761	−0.000169
3470.173	0.018946	−0.005778	0.002111	−0.000468
1514.523	0.047764	−0.014931	0.005482	−0.001220
689.5372	0.107998	−0.035345	0.013010	−0.002888
325.3052	0.208102	−0.075135	0.028068	−0.006266
158.2070	0.310027	−0.134205	0.051027	−0.011360
78.89893	0.296123	−0.177855	0.071027	−0.016033
39.86078	0.134623	−0.087706	0.036347	−0.008054
18.98692	0.016518	0.253945	−0.121697	0.027623
9.648207	−0.000198	0.551942	−0.380240	0.092886
4.916479	0.000417	0.328980	−0.323285	0.079434
2.283265	−0.000207	0.042135	0.299891	−0.085816
1.105562	0.000043	−0.000034	0.687190	−0.240295
0.514938	−0.000029	0.001079	0.309743	−0.229256
0.128805	0.000008	−0.000159	0.010895	0.338462
0.060049	−0.000006	0.000118	−0.004221	0.597949
0.027076	0.000002	−0.000037	0.001056	0.235250

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−22.365260	−2.248814		−0.569155
21569.96	0.000022	−0.000008	376.6631	0.000181
5104.709	0.000194	−0.000068	113.1116	0.001679
1658.134	0.001126	−0.000399	43.80518	0.009040
634.8811	0.005045	−0.001795	19.12971	0.032189
269.8101	0.018385	−0.006603	8.869862	0.086957
123.2384	0.055464	−0.020266	4.306251	0.179894
59.37291	0.135509	−0.051120	2.126995	0.271302
29.66752	0.254292	−0.099553	1.042759	0.311343
15.17617	0.342379	−0.142242	0.501614	0.269374
7.904346	0.274189	−0.103374	0.232462	0.152613
4.107973	0.096531	0.111608	0.099895	0.037557
2.089835	0.010127	0.376325		
1.037595	0.000999	0.432227		
0.499415	0.000111	0.216481		
0.206989	0.000030	0.026117		

Table CXXXV. Cr ^5D ($23s16p8d$) basis set. Energy(E_H) = -1043.309580.

	s space			
Exponent	1s	2s	3s	4s
	−220.592100	−26.439030	−3.498981	−0.239695
18856010.	0.000001	0.000000	0.000000	0.000000
2822858.	0.000009	−0.000003	0.000001	0.000000
642356.0	0.000046	−0.000014	0.000005	−0.000001
181947.3	0.000194	−0.000058	0.000021	−0.000005
59363.63	0.000708	−0.000212	0.000078	−0.000017
21434.29	0.002310	−0.000694	0.000253	−0.000056
8361.810	0.006892	−0.002083	0.000761	−0.000169
3469.432	0.018950	−0.005780	0.002111	−0.000468
1514.200	0.047776	−0.014935	0.005483	−0.001220
689.3896	0.108023	−0.035353	0.013013	−0.002888
325.2344	0.208140	−0.075151	0.028074	−0.006267
158.1718	0.310054	−0.134227	0.051036	−0.011361
78.88115	0.296090	−0.177857	0.071028	−0.016032
39.85205	0.134562	−0.087643	0.036321	−0.008049
18.98380	0.016502	0.254052	−0.121756	0.027635
9.646674	−0.000196	0.551943	−0.380278	0.092887
4.915819	0.000416	0.328882	−0.323194	0.079409
2.283069	−0.000207	0.042115	0.299973	−0.085841
1.105484	0.000043	−0.000033	0.687152	−0.240250
0.514916	−0.000029	0.001079	0.309707	−0.229250
0.128881	0.000008	−0.000159	0.010892	0.337754
0.060091	−0.000006	0.000118	−0.004211	0.598352
0.027082	0.000002	−0.000036	0.001052	0.235548

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−22.365160	−2.248713		−0.569044
31610.81	0.000011	−0.000004	118.3212	0.002098
7480.684	0.000099	−0.000035	35.21705	0.016189
2430.279	0.000582	−0.000206	13.06774	0.065493
930.9944	0.002645	−0.000940	5.352992	0.178306
396.2868	0.009907	−0.003538	2.302392	0.313616
181.5219	0.031232	−0.011301	0.981897	0.373302
87.78889	0.082610	−0.030567	0.403554	0.293086
44.22831	0.176089	−0.067469	0.151357	0.108150
22.88441	0.287692	−0.114677		
12.07596	0.329008	−0.139381		
6.447109	0.211982	−0.053036		
3.402996	0.057175	0.186892		
1.758967	0.004536	0.403343		
0.890848	0.000750	0.389054		
0.435736	0.000065	0.163655		
0.175970	0.000019	0.015614		

Table CXXXVI. Cr ^5D $(24s16p12d)$ basis set. Energy(E_H) = −1043.309804

	s space			
Exponent	1s	2s	3s	4s
	−220.592200	−26.439140	−3.499095	−0.239737
29807400.	0.000001	0.000000	0.000000	0.000000
4468122.	0.000005	−0.000002	0.000001	0.000000
1017735.	0.000026	−0.000008	0.000003	−0.000001
288465.7	0.000109	−0.000033	0.000012	−0.000003
94154.46	0.000398	−0.000119	0.000044	−0.000010
34003.23	0.001301	−0.000391	0.000143	−0.000032
13266.27	0.003896	−0.001173	0.000428	−0.000095
5504.435	0.010812	−0.003279	0.001199	−0.000267
2402.365	0.027838	−0.008562	0.003132	−0.000695
1093.899	0.065711	−0.020852	0.007665	−0.001707
516.2653	0.137994	−0.046517	0.017191	−0.003817
251.1334	0.242577	−0.092231	0.034642	−0.007743
125.3303	0.317708	−0.150796	0.058058	−0.012933
63.75407	0.250668	−0.168088	0.068173	−0.015460
32.65300	0.084122	−0.022810	0.009346	−0.001880
16.47243	0.006441	0.333002	−0.168780	0.038624
8.558107	0.000893	0.532982	−0.397788	0.098387
4.457992	−0.000200	0.261797	−0.253955	0.061177
2.141220	0.000056	0.029467	0.357229	−0.101370
1.049370	−0.000081	0.000895	0.664503	−0.240772
0.497818	0.000016	0.000696	0.279393	−0.216027
0.130285	−0.000007	−0.000058	0.009412	0.336646
0.060144	0.000005	0.000044	−0.003371	0.603337
0.027024	−0.000002	−0.000014	0.000834	0.234349

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−22.365270	−2.248818		−0.569159
31539.89	0.000011	−0.000004	548.5256	0.000080
7460.234	0.000100	−0.000035	165.0728	0.000765
2422.622	0.000586	−0.000207	63.98539	0.004399
927.7547	0.002662	−0.000946	28.23513	0.017203
394.8041	0.009971	−0.003561	13.30655	0.049762
180.8027	0.031428	−0.011373	6.549218	0.116069
87.42393	0.083091	−0.030750	3.325077	0.206462
44.03427	0.176936	−0.067813	1.696326	0.277788
22.77704	0.288599	−0.115076	0.856541	0.294064
12.01547	0.328958	−0.139406	0.424250	0.235706
6.411751	0.210648	−0.051510	0.202545	0.122857
3.381136	0.056205	0.189679	0.090063	0.027101
1.747054	0.004382	0.404511		
0.885004	0.000747	0.387203		
0.433028	0.000061	0.161466		
0.174529	0.000019	0.015226		

Table CXXXVII. Mn ^6S ($20s12p9d$) basis set. Energy(E_H) = -1149.865774

	s space			
Exponent	1s	2s	3s	4s
	−240.533900	−29.109370	−3.816551	−0.247829
3960805.	0.000009	−0.000003	0.000001	0.000000
593115.5	0.000068	−0.000020	0.000007	−0.000002
134976.8	0.000357	−0.000108	0.000040	−0.000009
38230.67	0.001507	−0.000455	0.000167	−0.000036
12471.54	0.005458	−0.001655	0.000608	−0.000132
4501.743	0.017500	−0.005358	0.001974	−0.000428
1755.212	0.049935	−0.015657	0.005776	−0.001253
727.3039	0.123881	−0.040951	0.015233	−0.003307
316.3678	0.250497	−0.092873	0.034921	−0.007592
143.0098	0.358959	−0.168424	0.065484	−0.014298
66.21805	0.275902	−0.189190	0.077032	−0.016914
29.91896	0.065959	0.046169	−0.019566	0.004279
14.30318	−0.001235	0.514709	−0.300536	0.069395
6.839451	0.001953	0.504200	−0.456340	0.110908
3.012374	−0.000903	0.091835	0.120444	−0.037390
1.418808	0.000393	−0.002551	0.727844	−0.227403
0.623624	−0.000155	0.002274	0.403565	−0.257984
0.134098	0.000059	−0.000519	0.016874	0.325997
0.065548	−0.000047	0.000417	−0.008309	0.568975
0.029584	0.000015	−0.000128	0.002102	0.263411

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−24.812470	−2.479438		−0.638760
7048.271	0.000178	−0.000064	199.8357	0.000901
1669.678	0.001567	−0.000561	59.72176	0.007668
541.8571	0.008715	−0.003147	22.74772	0.034658
206.4295	0.035717	−0.013040	9.565003	0.105774
86.89334	0.111212	−0.041923	4.285499	0.225939
39.06309	0.251615	−0.098570	1.950975	0.327657
18.24725	0.381207	−0.159635	0.872796	0.340005
8.741289	0.310341	−0.115053	0.375621	0.233804
4.119332	0.088028	0.177013	0.148009	0.073680
1.914804	0.003746	0.477435		
0.857893	0.001254	0.412634		
0.354950	−0.000102	0.099142		

Table CXXXVIII. Mn ^6S ($21s13p10d$) basis set. Energy(E_H) = −1149.866071

	s space			
Exponent	1s	2s	3s	4s
	−240.533900	−29.109430	−3.816608	−0.247852
6970524.	0.000004	−0.000001	0.000001	0.000000
1043706.	0.000034	−0.000010	0.000004	−0.000001
237516.7	0.000176	−0.000053	0.000020	−0.000004
67276.67	0.000745	−0.000225	0.000083	−0.000018
21948.82	0.002707	−0.000819	0.000301	−0.000065
7923.921	0.008765	−0.002665	0.000979	−0.000212
3090.491	0.025612	−0.007902	0.002916	−0.000633
1281.667	0.067116	−0.021319	0.007872	−0.001706
558.6622	0.152388	−0.051821	0.019352	−0.004207
253.5887	0.278167	−0.108120	0.040858	−0.008878
118.8854	0.348772	−0.178234	0.070140	−0.015362
56.64988	0.225217	−0.161422	0.066393	−0.014543
25.42406	0.041563	0.130614	−0.059155	0.012985
12.59866	−0.002310	0.545742	−0.342655	0.080246
6.195772	0.001721	0.431420	−0.407675	0.098765
2.761828	−0.000793	0.066716	0.210819	−0.060675
1.318391	0.000339	−0.001806	0.712761	−0.231671
0.594457	−0.000135	0.001791	0.355410	−0.240354
0.135225	0.000048	−0.000360	0.013278	0.338311
0.063784	−0.000036	0.000277	−0.005920	0.581977
0.028742	0.000011	−0.000087	0.001523	0.242372

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−24.812540	−2.479494		−0.638814
10868.06	0.000084	−0.000030	293.4870	0.000398
2573.534	0.000743	−0.000266	87.91274	0.003583
835.7456	0.004224	−0.001516	33.89617	0.017904
319.3070	0.018027	−0.006549	14.56697	0.059251
135.0114	0.060532	−0.022348	6.665463	0.146525
61.24025	0.157077	−0.060279	3.165037	0.256661
29.07445	0.297084	−0.118516	1.501904	0.324085
14.21473	0.369933	−0.158731	0.698724	0.303288
7.068309	0.233934	−0.052453	0.312725	0.187318
3.408898	0.049460	0.260979	0.128793	0.051605
1.615455	0.001632	0.481294		
0.743011	0.000799	0.345488		
0.311734	−0.000041	0.067441		

Table CXXXIX. Mn ^6S $(22s14p10d)$ basis set. Energy(E_H) = −1149.866161

	s space			
Exponent	1s	2s	3s	4s
	−240.534000	−29.109450	−3.816619	−0.247858
12210500.	0.000002	−0.000001	0.000000	0.000000
1828157.	0.000017	−0.000005	0.000002	0.000000
416030.3	0.000088	−0.000026	0.000010	−0.000002
117843.6	0.000370	−0.000112	0.000041	−0.000009
38448.14	0.001348	−0.000407	0.000149	−0.000032
13881.71	0.004386	−0.001330	0.000490	−0.000106
5415.002	0.012994	−0.003965	0.001458	−0.000316
2246.460	0.035119	−0.010928	0.004037	−0.000877
980.1463	0.085350	−0.027536	0.010185	−0.002207
445.8952	0.178688	−0.062587	0.023458	−0.005105
210.0558	0.296132	−0.121028	0.046008	−0.009997
101.8046	0.327547	−0.180987	0.071992	−0.015810
50.01126	0.181042	−0.129872	0.053891	−0.011768
22.93939	0.027732	0.194110	−0.091132	0.020113
11.52264	−0.001402	0.555273	−0.367851	0.086945
5.776338	0.001079	0.377854	−0.365411	0.088165
2.625959	−0.000500	0.052792	0.265346	−0.074904
1.260322	0.000189	−0.000795	0.699607	−0.233461
0.577130	−0.000081	0.001383	0.327031	−0.229429
0.136582	0.000027	−0.000241	0.011567	0.338645
0.063535	−0.000020	0.000181	−0.004817	0.589090
0.028521	0.000006	−0.000057	0.001232	0.237422

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−24.812560	−2.479506		−0.638823
16205.86	0.000042	−0.000015	293.4091	0.000398
3836.274	0.000372	−0.000133	87.88792	0.003585
1246.048	0.002143	−0.000769	33.88644	0.017912
476.7535	0.009416	−0.003397	14.56257	0.059280
202.1895	0.033193	−0.012147	6.662674	0.146627
92.09487	0.094455	−0.035435	3.162963	0.256835
44.14720	0.207445	−0.080936	1.500646	0.324141
21.85468	0.330672	−0.135286	0.698180	0.303128
11.08596	0.332028	−0.141132	0.312565	0.187148
5.674108	0.157864	0.026936	0.128747	0.051569
2.823170	0.024226	0.328554		
1.368621	0.001256	0.464875		
0.644431	0.000364	0.279803		
0.271218	0.000021	0.043773		

Table CXL. Mn ^6S $(22s15p11d)$ basis set. Energy(E_H) = −1149.866197

	s space			
Exponent	1s	2s	3s	4s
	−240.534000	−29.109460	−3.816632	−0.247865
12216120.	0.000002	−0.000001	0.000000	0.000000
1828917.	0.000017	−0.000005	0.000002	0.000000
416195.5	0.000088	−0.000026	0.000010	−0.000002
117889.8	0.000370	−0.000112	0.000041	−0.000009
38462.87	0.001347	−0.000407	0.000149	−0.000032
13886.72	0.004384	−0.001330	0.000489	−0.000106
5416.786	0.012989	−0.003964	0.001457	−0.000316
2247.127	0.035108	−0.010925	0.004036	−0.000876
980.4106	0.085328	−0.027529	0.010182	−0.002207
446.0052	0.178655	−0.062572	0.023452	−0.005104
210.1016	0.296112	−0.121013	0.046003	−0.009996
101.8229	0.327580	−0.180984	0.071989	−0.015809
50.01849	0.181086	−0.129924	0.053913	−0.011774
22.94618	0.027745	0.193949	−0.091051	0.020096
11.52552	−0.001396	0.555250	−0.367768	0.086921
5.777639	0.001076	0.377992	−0.365561	0.088209
2.626912	−0.000499	0.052839	0.265060	−0.074835
1.260669	0.000188	−0.000789	0.699703	−0.233446
0.577235	−0.000081	0.001383	0.327196	−0.229521
0.136669	0.000027	−0.000241	0.011572	0.337951
0.063610	−0.000020	0.000181	−0.004812	0.589028
0.028553	0.000006	−0.000057	0.001231	0.238179

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−24.812580	−2.479519		−0.638835
23797.17	0.000021	−0.000008	424.5513	0.000180
5631.601	0.000191	−0.000068	127.5869	0.001674
1829.258	0.001109	−0.000398	49.44855	0.009088
700.4122	0.004973	−0.001789	21.63556	0.032677
297.6977	0.018161	−0.006597	10.06210	0.088577
136.0188	0.054947	−0.020309	4.897678	0.182725
65.56236	0.134758	−0.051448	2.424570	0.273864
32.78773	0.253993	−0.100738	1.190693	0.310957
16.79460	0.342767	−0.144281	0.573136	0.265916
8.759732	0.274367	−0.103526	0.265552	0.148976
4.558713	0.096656	0.114719	0.113774	0.036248
2.322083	0.010303	0.378036		
1.153402	0.001076	0.429653		
0.555009	0.000141	0.215295		
0.231018	0.000035	0.026265		

Table CXLI. Mn ^6S $(23s15p11d)$ basis set. Energy(E_H) = −1149.866215

	s space			
Exponent	1s	2s	3s	4s
	−240.534000	−29.109460	−3.816635	−0.247865
20492660.	0.000001	0.000000	0.000000	0.000000
3068183.	0.000009	−0.000003	0.000001	0.000000
698235.9	0.000046	−0.000014	0.000005	−0.000001
197786.6	0.000194	−0.000058	0.000021	−0.000005
64534.02	0.000706	−0.000213	0.000079	−0.000017
23301.75	0.002306	−0.000697	0.000256	−0.000055
9090.491	0.006880	−0.002092	0.000770	−0.000167
3771.821	0.018920	−0.005806	0.002136	−0.000463
1646.193	0.047709	−0.015007	0.005550	−0.001206
749.5010	0.107909	−0.035543	0.013181	−0.002856
353.6151	0.208029	−0.075622	0.028464	−0.006202
171.9954	0.310064	−0.135204	0.051826	−0.011263
85.79538	0.296249	−0.179232	0.072188	−0.015905
43.37356	0.134628	−0.087887	0.036826	−0.007972
20.70091	0.016458	0.258017	−0.125719	0.027899
10.54152	−0.000216	0.553621	−0.387901	0.092519
5.379760	0.000402	0.325132	−0.317770	0.076094
2.504388	−0.000201	0.041251	0.313107	−0.087471
1.209910	0.000041	0.000120	0.684599	−0.234365
0.561918	−0.000028	0.001025	0.302400	−0.219495
0.137924	0.000008	−0.000141	0.010263	0.337148
0.063563	−0.000005	0.000105	−0.004017	0.594367
0.028436	0.000002	−0.000033	0.001019	0.235786

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−24.812580	−2.479521		−0.638837
23784.73	0.000021	−0.000008	424.6654	0.000179
5628.802	0.000191	−0.000068	127.6252	0.001673
1828.374	0.001110	−0.000398	49.46356	0.009083
700.0849	0.004977	−0.001790	21.64174	0.032664
297.5632	0.018174	−0.006601	10.06476	0.088549
135.9586	0.054982	−0.020322	4.898980	0.182682
65.53392	0.134823	−0.051473	2.425242	0.273836
32.77452	0.254054	−0.100765	1.191026	0.310959
16.78867	0.342762	−0.144284	0.573302	0.265952
8.756926	0.274282	−0.103463	0.265628	0.149033
4.557208	0.096584	0.114871	0.113801	0.036272
2.321136	0.010287	0.378186		
1.152868	0.001076	0.429587		
0.554762	0.000141	0.215112		
0.230912	0.000035	0.026225		

Table CXLII. Mn ^6S $(23s16p8d)$ basis set. Energy(E_H) = −1149.865928 .

	s space			
Exponent	1s	2s	3s	4s
	−240.533900	−29.109340	−3.816497	−0.247815
20494330.	0.000001	0.000000	0.000000	0.000000
3068261.	0.000009	−0.000003	0.000001	0.000000
698199.6	0.000046	−0.000014	0.000005	−0.000001
197762.5	0.000194	−0.000058	0.000021	−0.000005
64522.83	0.000707	−0.000213	0.000079	−0.000017
23296.84	0.002307	−0.000697	0.000256	−0.000055
9088.316	0.006882	−0.002093	0.000771	−0.000167
3770.831	0.018927	−0.005808	0.002137	−0.000463
1645.730	0.047725	−0.015013	0.005552	−0.001206
749.2773	0.107945	−0.035556	0.013186	−0.002857
353.5033	0.208087	−0.075647	0.028474	−0.006203
171.9383	0.310107	−0.135238	0.051840	−0.011265
85.76604	0.296202	−0.179237	0.072191	−0.015904
43.35893	0.134535	−0.087787	0.036786	−0.007963
20.69503	0.016434	0.258205	−0.125825	0.027922
10.53854	−0.000213	0.553630	−0.387973	0.092528
5.378399	0.000401	0.324956	−0.317603	0.076048
2.504018	−0.000201	0.041213	0.313254	−0.087510
1.209767	0.000041	0.000123	0.684525	−0.234314
0.561884	−0.000027	0.001023	0.302345	−0.219468
0.137988	0.000008	−0.000141	0.010262	0.336495
0.063606	−0.000005	0.000105	−0.004010	0.594696
0.028442	0.000002	−0.000033	0.001014	0.236095

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−24.812450	−2.479392		−0.638695
35002.46	0.000011	−0.000004	133.6941	0.002086
8281.663	0.000097	−0.000035	39.83511	0.016265
2690.015	0.000570	−0.000204	14.83355	0.066423
1030.325	0.002592	−0.000931	6.100341	0.180745
438.5246	0.009730	−0.003514	2.632400	0.316253
200.8793	0.030767	−0.011259	1.125484	0.372416
97.17000	0.081702	−0.030583	0.462944	0.289132
48.97550	0.175036	−0.067884	0.173449	0.105689
25.36332	0.287375	−0.116089		
13.40145	0.329511	−0.141167		
7.164560	0.212701	−0.052713		
3.787859	0.057731	0.188995		
1.960350	0.004752	0.403407		
0.992856	0.000810	0.387104		
0.485484	0.000091	0.163896		
0.197241	0.000022	0.015857		

Table CXLIII. Mn ^6S $(24s16p12d)$ basis set. Energy(E_H) = −1149.866235

	s space			
Exponent	1s	2s	3s	4s
	−240.534000	−29.109470	−3.816641	−0.247868
32461360.	0.000001	0.000000	0.000000	0.000000
4861222.	0.000005	−0.000002	0.000001	0.000000
1106616.	0.000026	−0.000008	0.000003	−0.000001
313549.3	0.000109	−0.000033	0.000012	−0.000003
102321.8	0.000397	−0.000120	0.000044	−0.000010
36950.07	0.001299	−0.000393	0.000144	−0.000031
14416.25	0.003891	−0.001179	0.000433	−0.000094
5982.058	0.010798	−0.003295	0.001213	−0.000263
2611.120	0.027800	−0.008603	0.003170	−0.000686
1189.127	0.065622	−0.020956	0.007760	−0.001687
561.3166	0.137836	−0.046767	0.017414	−0.003773
273.1242	0.242380	−0.092797	0.035122	−0.007662
136.3583	0.317632	−0.151821	0.058940	−0.012817
69.40586	0.250873	−0.169345	0.069282	−0.015335
35.59082	0.084339	−0.022539	0.009366	−0.001842
17.97997	0.006457	0.337157	−0.173873	0.038900
9.357553	0.000853	0.533484	−0.404255	0.097596
4.879581	−0.000196	0.258444	−0.246723	0.057834
2.348285	0.000052	0.028866	0.368842	−0.102289
1.149027	−0.000076	0.000981	0.660823	−0.234323
0.543550	0.000015	0.000665	0.273084	−0.206863
0.139387	−0.000007	−0.000049	0.008906	0.335502
0.063659	0.000005	0.000039	−0.003242	0.599203
0.028389	−0.000001	−0.000012	0.000814	0.235025

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−24.812580	−2.479526		−0.638842
35005.12	0.000011	−0.000004	605.5824	0.000083
8279.462	0.000097	−0.000035	182.5636	0.000793
2688.465	0.000571	−0.000204	70.88019	0.004562
1029.490	0.002596	−0.000933	31.34585	0.017870
438.0708	0.009749	−0.003521	14.82938	0.051678
200.6153	0.030841	−0.011287	7.334336	0.119635
97.00769	0.081932	−0.030670	3.738981	0.210491
48.87052	0.175560	−0.068098	1.913749	0.279829
25.29281	0.288152	−0.116422	0.968462	0.291950
13.35382	0.329797	−0.141326	0.480219	0.230471
7.131786	0.211826	−0.051459	0.229364	0.118102
3.764365	0.056864	0.191891	0.101771	0.025550
1.946265	0.004585	0.404953		
0.985455	0.000809	0.385249		
0.481865	0.000085	0.161382		
0.195171	0.000023	0.015362		

Table CXLIV. Fe ^5D $(20s12p9d)$ basis set. Energy(E_H) = −1262.443122 .

	s space			
Exponent	1s	2s	3s	4s
	−261.373300	−31.935390	−4.169324	−0.258131
4316265.	0.000009	−0.000003	0.000001	0.000000
646342.4	0.000067	−0.000020	0.000008	−0.000002
147089.7	0.000354	−0.000108	0.000040	−0.000008
41661.52	0.001494	−0.000454	0.000168	−0.000036
13590.77	0.005411	−0.001650	0.000611	−0.000131
4905.750	0.017353	−0.005342	0.001984	−0.000424
1912.746	0.049540	−0.015619	0.005806	−0.001242
792.6043	0.123034	−0.040888	0.015328	−0.003284
344.8065	0.249291	−0.092907	0.035210	−0.007552
155.8999	0.358569	−0.168937	0.066225	−0.014271
72.23091	0.277479	−0.190991	0.078452	−0.016995
32.72506	0.067201	0.043968	−0.018786	0.004039
15.66762	−0.001155	0.515453	−0.305186	0.069618
7.503483	0.001932	0.505163	−0.459335	0.110089
3.312223	−0.000892	0.092375	0.127054	−0.038479
1.558471	0.000385	−0.002403	0.729233	−0.226185
0.683914	−0.000151	0.002245	0.399261	−0.250673
0.146757	0.000056	−0.000493	0.016524	0.319752
0.070583	−0.000044	0.000391	−0.007960	0.570895
0.031449	0.000014	−0.000121	0.002026	0.266004

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−27.413570	−2.742084		−0.646780
7721.489	0.000177	−0.000064	217.3688	0.000945
1829.126	0.001551	−0.000562	64.99976	0.008059
593.6280	0.008639	−0.003156	24.77314	0.036510
226.2054	0.035483	−0.013109	10.43614	0.111013
95.26145	0.110802	−0.042284	4.679653	0.232606
42.85920	0.251546	−0.099848	2.125622	0.329231
20.04971	0.381644	−0.162055	0.945242	0.334776
9.620885	0.309961	−0.114943	0.402685	0.229867
4.541371	0.087770	0.181703	0.156651	0.074367
2.113500	0.003863	0.479484		
0.947201	0.001285	0.408551		
0.391243	−0.000077	0.097359		

Table CXLV. Fe ^5D ($21s13p10d$) basis set. Energy(E_H) = −1262.443462

	s space			
Exponent	1s	2s	3s	4s
	−261.373400	−31.935470	−4.169394	−0.258159
7585273.	0.000004	−0.000001	0.000001	0.000000
1135752.	0.000033	−0.000010	0.000004	−0.000001
258462.3	0.000175	−0.000053	0.000020	−0.000004
73208.99	0.000740	−0.000224	0.000083	−0.000018
23884.05	0.002688	−0.000818	0.000303	−0.000065
8622.519	0.008706	−0.002662	0.000986	−0.000211
3362.940	0.025445	−0.007895	0.002935	−0.000629
1394.654	0.066716	−0.021310	0.007930	−0.001696
607.9274	0.151647	−0.051851	0.019514	−0.004186
275.9750	0.277342	−0.108383	0.041287	−0.008852
129.4041	0.348890	−0.179114	0.071074	−0.015363
61.69321	0.226561	−0.163173	0.067753	−0.014644
27.74665	0.042189	0.129995	−0.059665	0.012922
13.78241	−0.002350	0.547044	−0.348373	0.080590
6.789430	0.001725	0.431293	−0.408601	0.097615
3.035275	−0.000793	0.066889	0.218361	−0.061781
1.447451	0.000337	−0.001657	0.713110	−0.230137
0.651559	−0.000133	0.001757	0.351106	−0.233072
0.147876	0.000046	−0.000339	0.013040	0.331626
0.068785	−0.000035	0.000258	−0.005693	0.582667
0.030611	0.000011	−0.000081	0.001471	0.246459

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−27.413660	−2.742154		−0.646847
11900.61	0.000083	−0.000030	318.6382	0.000419
2817.990	0.000736	−0.000267	95.49585	0.003776
915.1351	0.004188	−0.001521	36.83605	0.018897
349.6766	0.017903	−0.006581	15.84522	0.062605
147.8969	0.060261	−0.022519	7.262604	0.153042
67.11805	0.156845	−0.060947	3.446759	0.262102
31.89385	0.297480	−0.120332	1.630302	0.323137
15.61608	0.370200	−0.160826	0.753400	0.297416
7.776964	0.233176	−0.050658	0.333897	0.184325
3.758304	0.049231	0.265779	0.135919	0.052234
1.783213	0.001752	0.481751		
0.820137	0.000822	0.341321		
0.343476	−0.000021	0.066184		

Table CXLVI. Fe ^5D ($22s14p10d$) basis set. Energy(E_H) = -1262.443559

	s space			
Exponent	1s	2s	3s	4s
	−261.373400	−31.935490	−4.169406	−0.258165
13277210.	0.000002	−0.000001	0.000000	0.000000
1987840.	0.000016	−0.000005	0.000002	0.000000
452364.6	0.000087	−0.000026	0.000010	−0.000002
128134.6	0.000368	−0.000112	0.000041	−0.000009
41805.71	0.001340	−0.000407	0.000151	−0.000032
15094.05	0.004360	−0.001330	0.000493	−0.000106
5887.968	0.012919	−0.003964	0.001469	−0.000314
2442.703	0.034926	−0.010929	0.004068	−0.000872
1065.789	0.084930	−0.027554	0.010271	−0.002196
484.8808	0.178007	−0.062695	0.023682	−0.005086
228.4453	0.295555	−0.121457	0.046551	−0.009981
110.7389	0.327933	−0.182069	0.073033	−0.015829
54.42804	0.182160	−0.131391	0.055079	−0.011868
25.01037	0.028089	0.194746	−0.092775	0.020214
12.59209	−0.001449	0.556661	−0.374090	0.087337
6.322880	0.001083	0.376895	−0.364595	0.086728
2.883222	−0.000502	0.052724	0.273596	−0.076065
1.382827	0.000189	−0.000664	0.699153	−0.231722
0.632212	−0.000080	0.001351	0.322584	−0.222096
0.149244	0.000026	−0.000224	0.011356	0.332398
0.068504	−0.000019	0.000167	−0.004633	0.589045
0.030386	0.000006	−0.000052	0.001190	0.241705

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−27.413680	−2.742167		−0.646857
17745.69	0.000041	−0.000015	318.5459	0.000419
4200.721	0.000368	−0.000133	95.46847	0.003778
1364.429	0.002123	−0.000771	36.82577	0.018906
522.0806	0.009343	−0.003411	15.84068	0.062633
221.4595	0.033002	−0.012221	7.259779	0.153138
100.9096	0.094154	−0.035759	3.444646	0.262266
48.40115	0.207436	−0.081984	1.628987	0.323195
23.98536	0.331294	−0.137489	0.752807	0.297273
12.18250	0.331946	−0.142296	0.333713	0.184157
6.242298	0.157105	0.030335	0.135867	0.052194
3.110944	0.024085	0.333003		
1.509958	0.001342	0.463692		
0.710845	0.000388	0.275681		
0.298642	0.000035	0.042897		

Table CXLVII. Fe ^5D $(22s15p11d)$ basis set. Energy(E_H) = −1262.443604

	s space			
Exponent	1s	2s	3s	4s
	−261.373400	−31.935500	−4.169423	−0.258174
13277140.	0.000002	−0.000001	0.000000	0.000000
1987888.	0.000016	−0.000005	0.000002	0.000000
452387.1	0.000087	−0.000026	0.000010	−0.000002
128143.7	0.000368	−0.000112	0.000041	−0.000009
41809.17	0.001339	−0.000407	0.000151	−0.000032
15095.33	0.004360	−0.001330	0.000493	−0.000106
5888.438	0.012917	−0.003964	0.001469	−0.000314
2442.876	0.034923	−0.010928	0.004068	−0.000872
1065.857	0.084925	−0.027552	0.010270	−0.002196
484.9096	0.177998	−0.062692	0.023681	−0.005086
228.4585	0.295547	−0.121451	0.046549	−0.009980
110.7453	0.327937	−0.182067	0.073031	−0.015829
54.43116	0.182178	−0.131402	0.055083	−0.011869
25.01096	0.028096	0.194720	−0.092762	0.020211
12.59262	−0.001451	0.556643	−0.374067	0.087333
6.323202	0.001084	0.376923	−0.364623	0.086734
2.883384	−0.000502	0.052736	0.273548	−0.076049
1.382868	0.000189	−0.000664	0.699192	−0.231743
0.632201	−0.000080	0.001351	0.322591	−0.222097
0.149238	0.000026	−0.000224	0.011344	0.332487
0.068494	−0.000019	0.000167	−0.004623	0.589074
0.030381	0.000006	−0.000052	0.001188	0.241595

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−27.413700	−2.742184		−0.646873
26063.03	0.000021	−0.000008	460.2520	0.000190
6168.017	0.000189	−0.000068	138.3811	0.001769
2003.526	0.001098	−0.000398	53.65726	0.009609
767.1618	0.004929	−0.001794	23.48782	0.034602
326.1070	0.018031	−0.006628	10.93939	0.093463
149.0380	0.054682	−0.020456	5.329363	0.189419
71.86738	0.134490	−0.051991	2.634463	0.277336
35.96714	0.254232	−0.102205	1.288662	0.307940
18.44544	0.343262	−0.146485	0.615926	0.260164
9.632871	0.273930	−0.103314	0.282708	0.146911
5.018510	0.096154	0.119054	0.119845	0.036838
2.559184	0.010302	0.381471		
1.272210	0.001133	0.427102		
0.611926	0.000167	0.211628		
0.254299	0.000044	0.025733		

Table CXLVIII. Fe ^5D $(23s15p11d)$ basis set. Energy(E_H) $= -1262.443623$

	s space			
Exponent	1s	2s	3s	4s
	−261.373400	−31.935510	−4.169426	−0.258174
22219490.	0.000001	0.000000	0.000000	0.000000
3328111.	0.000009	−0.000003	0.000001	0.000000
757610.9	0.000046	−0.000014	0.000005	−0.000001
214653.0	0.000193	−0.000059	0.000022	−0.000005
70049.96	0.000704	−0.000214	0.000079	−0.000017
25297.35	0.002297	−0.000698	0.000259	−0.000055
9870.354	0.006851	−0.002095	0.000777	−0.000167
4095.895	0.018840	−0.005814	0.002156	−0.000461
1787.833	0.047514	−0.015030	0.005601	−0.001201
814.0833	0.107524	−0.035618	0.013312	−0.002846
384.1415	0.207486	−0.075859	0.028778	−0.006187
186.8802	0.309751	−0.135839	0.052507	−0.011259
93.24859	0.296746	−0.180454	0.073303	−0.015941
47.17213	0.135401	−0.088913	0.037678	−0.008048
22.55251	0.016614	0.259910	−0.128632	0.028190
11.50798	−0.000249	0.554797	−0.394341	0.092903
5.881659	0.000401	0.323413	−0.315042	0.074336
2.746291	−0.000201	0.040996	0.322033	−0.088705
1.326378	0.000041	0.000226	0.683241	−0.232430
0.615117	−0.000027	0.000996	0.297703	−0.212049
0.150577	0.000007	−0.000128	0.010062	0.331602
0.068486	−0.000005	0.000095	−0.003858	0.593757
0.030288	0.000002	−0.000030	0.000983	0.239851

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−27.413700	−2.742185		−0.646875
26045.28	0.000021	−0.000008	460.4508	0.000189
6164.157	0.000189	−0.000068	138.4285	0.001768
2002.388	0.001099	−0.000399	53.67183	0.009605
766.7725	0.004933	−0.001796	23.49262	0.034595
325.9611	0.018043	−0.006632	10.94070	0.093459
148.9799	0.054709	−0.020466	5.329644	0.189427
71.84373	0.134528	−0.052007	2.634448	0.277360
35.95811	0.254249	−0.102213	1.288586	0.307955
18.44234	0.343234	−0.146475	0.615881	0.260152
9.631793	0.273886	−0.103286	0.282691	0.146898
5.018068	0.096132	0.119097	0.119840	0.036833
2.558852	0.010299	0.381534		
1.271985	0.001133	0.427087		
0.611817	0.000167	0.211554		
0.254256	0.000044	0.025718		

Table CXLIX. Fe ^5D $(23s16p8d)$ basis set. Energy(E_H) = −1262.443211

	s space			
Exponent	1s	2s	3s	4s
	−261.373300	−31.935330	−4.169231	−0.258103
22200400.	0.000001	0.000000	0.000000	0.000000
3325132.	0.000009	−0.000003	0.000001	0.000000
756943.4	0.000046	−0.000014	0.000005	−0.000001
214470.4	0.000193	−0.000059	0.000022	−0.000005
69992.62	0.000704	−0.000214	0.000079	−0.000017
25277.43	0.002299	−0.000699	0.000259	−0.000055
9862.839	0.006857	−0.002097	0.000778	−0.000167
4092.882	0.018856	−0.005819	0.002158	−0.000461
1786.571	0.047551	−0.015042	0.005606	−0.001202
813.5370	0.107593	−0.035642	0.013322	−0.002848
383.8988	0.207579	−0.075903	0.028795	−0.006190
186.7722	0.309786	−0.135880	0.052524	−0.011262
93.20307	0.296625	−0.180437	0.073300	−0.015938
47.15543	0.135283	−0.088756	0.037610	−0.008032
22.54071	0.016598	0.260219	−0.128804	0.028225
11.50271	−0.000257	0.554761	−0.394450	0.092921
5.879457	0.000404	0.323158	−0.314715	0.074244
2.744773	−0.000203	0.040942	0.322430	−0.088805
1.325847	0.000042	0.000215	0.683041	−0.232375
0.614961	−0.000027	0.000999	0.297488	−0.211939
0.150619	0.000007	−0.000129	0.010051	0.331145
0.068502	−0.000005	0.000096	−0.003846	0.594210
0.030277	0.000002	−0.000030	0.000977	0.239840

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−27.413520	−2.742003		−0.646674
38282.05	0.000011	−0.000004	145.7437	0.002180
9061.556	0.000096	−0.000035	43.45268	0.017044
2944.450	0.000565	−0.000204	16.20179	0.069747
1128.158	0.002568	−0.000934	6.677760	0.187455
480.3380	0.009648	−0.003526	2.878893	0.320420
220.1368	0.030556	−0.011316	1.224827	0.368744
106.5482	0.081314	−0.030812	0.498728	0.284231
53.74262	0.174707	−0.068625	0.184268	0.106380
27.86318	0.287567	−0.117800		
14.74382	0.329680	−0.142923		
7.893351	0.212414	−0.051567		
4.179497	0.057683	0.192740		
2.165669	0.004855	0.405218		
1.097240	0.000854	0.384346		
0.536085	0.000116	0.161495		
0.217604	0.000028	0.015656		

Table CL. Fe ^5D $(24s16p12d)$ basis set. Energy(E_H) = −1262.443647

	s space			
Exponent	1s	2s	3s	4s
	−261.373400	−31.935510	−4.169433	−0.258177
35278030.	0.000001	0.000000	0.000000	0.000000
5279617.	0.000005	−0.000002	0.000001	0.000000
1201358.	0.000026	−0.000008	0.000003	−0.000001
340282.0	0.000109	−0.000033	0.000012	−0.000003
111022.5	0.000396	−0.000120	0.000044	−0.000010
40087.64	0.001295	−0.000394	0.000146	−0.000031
15639.52	0.003880	−0.001182	0.000438	−0.000094
6489.430	0.010767	−0.003304	0.001226	−0.000263
2832.451	0.027725	−0.008628	0.003204	−0.000684
1289.820	0.065478	−0.021029	0.007846	−0.001683
608.7813	0.137636	−0.046975	0.017631	−0.003770
296.1832	0.242270	−0.093328	0.035605	−0.007665
147.8496	0.317832	−0.152916	0.059882	−0.012849
75.24241	0.251259	−0.170638	0.070438	−0.015390
38.57524	0.084301	−0.021874	0.009224	−0.001778
19.53789	0.006318	0.341463	−0.179217	0.039610
10.18480	0.000871	0.533719	−0.410584	0.097924
5.316822	−0.000220	0.254972	−0.240139	0.055328
2.566845	0.000063	0.028255	0.379646	−0.103927
1.256224	−0.000079	0.001068	0.657715	−0.232192
0.593725	0.000017	0.000636	0.267142	−0.198879
0.152123	−0.000007	−0.000039	0.008654	0.330409
0.068559	0.000005	0.000032	−0.003071	0.598380
0.030227	−0.000001	−0.000010	0.000774	0.238847

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−27.413700	−2.742192		−0.646882
37465.18	0.000011	−0.000004	672.8062	0.000083
8875.622	0.000100	−0.000036	202.3609	0.000801
2886.188	0.000584	−0.000212	78.43251	0.004650
1106.538	0.002652	−0.000964	34.63383	0.018401
471.3946	0.009942	−0.003634	16.36345	0.053714
216.1431	0.031398	−0.011633	8.083712	0.124149
104.6624	0.083226	−0.031560	4.111713	0.215491
52.80791	0.177790	−0.069909	2.096818	0.281183
27.38145	0.290410	−0.119131	1.055175	0.288404
14.49039	0.328811	−0.142613	0.519028	0.226758
7.755196	0.207641	−0.046361	0.245468	0.118159
4.100813	0.054694	0.200744	0.107712	0.026587
2.124170	0.004436	0.407935		
1.077138	0.000834	0.378963		
0.526821	0.000107	0.155533		
0.212744	0.000027	0.014596		

Table CLI. Co ^4F $(20s12p9d)$ basis set. Energy(E_H) = −1381.413937

	s space			
Exponent	1s	2s	3s	4s
	−283.065300	−34.868190	−4.524152	−0.267363
4676708.	0.000009	−0.000003	0.000001	0.000000
700317.2	0.000067	−0.000020	0.000008	−0.000002
159373.0	0.000352	−0.000108	0.000040	−0.000008
45140.67	0.001486	−0.000454	0.000169	−0.000036
14725.75	0.005383	−0.001650	0.000615	−0.000129
5315.448	0.017265	−0.005342	0.001996	−0.000420
2072.498	0.049304	−0.015624	0.005843	−0.001230
858.8231	0.122536	−0.040929	0.015439	−0.003255
373.6437	0.248604	−0.093128	0.035517	−0.007496
168.9682	0.358379	−0.169654	0.066957	−0.014201
78.31971	0.278411	−0.192452	0.079625	−0.016972
35.53724	0.067858	0.043475	−0.018742	0.003957
17.04735	−0.001156	0.517362	−0.310374	0.069742
8.175534	0.001921	0.504662	−0.460632	0.108565
3.611578	−0.000886	0.091988	0.136059	−0.040094
1.697468	0.000381	−0.002313	0.729895	−0.223807
0.743636	−0.000148	0.002212	0.393620	−0.242984
0.158325	0.000053	−0.000470	0.015975	0.317066
0.075009	−0.000042	0.000370	−0.007605	0.571008
0.033093	0.000013	−0.000115	0.001957	0.266512

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−30.120010	−3.006110		−0.675290
8421.842	0.000175	−0.000064	237.5928	0.000971
1995.000	0.001538	−0.000562	71.08881	0.008301
647.4855	0.008574	−0.003163	27.11903	0.037770
246.7795	0.035291	−0.013165	11.44826	0.114649
103.9689	0.110483	−0.042589	5.139542	0.237214
46.81052	0.251572	−0.100952	2.332694	0.330389
21.92703	0.382065	−0.164106	1.034030	0.331148
10.53715	0.309508	−0.114594	0.437899	0.226607
4.980678	0.087479	0.185823	0.168963	0.074277
2.319824	0.003972	0.480768		
1.039609	0.001316	0.405132		
0.428921	−0.000057	0.096190		

Table CLII. Co ^4F $(19s12p8d)$ basis set. Energy(E_H) = −1381.413447

	s space			
Exponent	1s	2s	3s	4s
	−283.065100	−34.867930	−4.523895	−0.267209
4618025.	0.000009	−0.000003	0.000001	0.000000
691531.1	0.000068	−0.000021	0.000008	−0.000002
157373.5	0.000358	−0.000109	0.000041	−0.000008
44574.26	0.001510	−0.000461	0.000172	−0.000036
14540.94	0.005467	−0.001676	0.000625	−0.000131
5248.718	0.017532	−0.005426	0.002027	−0.000428
2046.465	0.050032	−0.015860	0.005932	−0.001245
848.0186	0.124145	−0.041521	0.015665	−0.003312
368.9246	0.251037	−0.094256	0.035960	−0.007552
166.8100	0.359359	−0.171099	0.067572	−0.014414
77.26387	0.275425	−0.191274	0.079239	−0.016658
34.86393	0.065084	0.052234	−0.022873	0.004274
16.78474	−0.001563	0.524296	−0.317039	0.072607
8.055614	0.001958	0.496254	−0.456308	0.104911
3.551150	−0.000880	0.086902	0.156084	−0.039735
1.662265	0.000355	−0.001911	0.734254	−0.237749
0.723875	−0.000122	0.001858	0.378306	−0.223619
0.124743	0.000022	−0.000183	0.008933	0.600370
0.044239	−0.000009	0.000077	−0.002525	0.546075

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−30.119760	−3.005865		−0.675025
8430.984	0.000175	−0.000064	159.4898	0.002236
1997.162	0.001535	−0.000561	47.58167	0.017557
648.1878	0.008559	−0.003157	17.77066	0.072090
247.0492	0.035231	−0.013143	7.340541	0.192186
104.0830	0.110325	−0.042526	3.164879	0.323427
46.86201	0.251323	−0.100847	1.343309	0.366218
21.95154	0.381940	−0.164026	0.543916	0.280241
10.54945	0.309795	−0.114876	0.199336	0.106122
4.987676	0.087760	0.185128		
2.323129	0.004013	0.480568		
1.040946	0.001315	0.405717		
0.429412	−0.000056	0.096501		

Table CLIII. Co ^4F $(20s12p8d)$ basis set. Energy(E_H) = −1381.413522

	s space			
Exponent	1s	2s	3s	4s
	−283.065200	−34.868020	−4.523973	−0.267298
4677513.	0.000009	−0.000003	0.000001	0.000000
700439.9	0.000067	−0.000020	0.000008	−0.000002
159401.6	0.000352	−0.000108	0.000040	−0.000008
45149.02	0.001486	−0.000454	0.000169	−0.000036
14728.55	0.005381	−0.001650	0.000615	−0.000129
5316.482	0.017261	−0.005341	0.001995	−0.000420
2072.910	0.049292	−0.015620	0.005842	−0.001230
858.9980	0.122509	−0.040919	0.015436	−0.003254
373.7216	0.248563	−0.093109	0.035509	−0.007494
169.0044	0.358361	−0.169630	0.066946	−0.014196
78.33757	0.278460	−0.192471	0.079632	−0.016972
35.54877	0.067905	0.043328	−0.018677	0.003944
17.05200	−0.001148	0.517227	−0.310239	0.069699
8.177834	0.001919	0.504797	−0.460715	0.108577
3.613146	−0.000885	0.092086	0.135675	−0.040000
1.698092	0.000380	−0.002306	0.729889	−0.223720
0.743857	−0.000148	0.002213	0.393892	−0.243054
0.158398	0.000053	−0.000470	0.016016	0.316118
0.075111	−0.000042	0.000371	−0.007625	0.571098
0.033119	0.000013	−0.000115	0.001957	0.267313

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−30.119850	−3.005941		−0.675101
8432.219	0.000174	−0.000064	159.4861	0.002237
1997.459	0.001535	−0.000561	47.58053	0.017558
648.2864	0.008557	−0.003156	17.77018	0.072092
247.0878	0.035223	−0.013140	7.340307	0.192193
104.0999	0.110301	−0.042516	3.164749	0.323433
46.87001	0.251282	−0.100830	1.343255	0.366213
21.95546	0.381918	−0.164013	0.543867	0.280254
10.55143	0.309841	−0.114921	0.199310	0.106106
4.988796	0.087806	0.185018		
2.323643	0.004020	0.480539		
1.041198	0.001315	0.405772		
0.429543	−0.000056	0.096587		

Table CLIV. Co ^4F $(20s13p8d)$ basis set. Energy(E_H) = −1381.413689

	s space			
Exponent	1s	2s	3s	4s
	−283.065200	−34.868040	−4.523988	−0.267310
4675675.	0.000009	−0.000003	0.000001	0.000000
700161.5	0.000067	−0.000020	0.000008	−0.000002
159337.3	0.000353	−0.000108	0.000040	−0.000008
45130.46	0.001487	−0.000454	0.000169	−0.000036
14722.38	0.005384	−0.001651	0.000615	−0.000129
5314.222	0.017270	−0.005343	0.001997	−0.000420
2072.018	0.049317	−0.015628	0.005845	−0.001231
858.6188	0.122567	−0.040940	0.015444	−0.003256
373.5497	0.248656	−0.093152	0.035526	−0.007497
168.9229	0.358406	−0.169687	0.066972	−0.014203
78.29639	0.278352	−0.192432	0.079617	−0.016969
35.52123	0.067796	0.043673	−0.018832	0.003975
17.04144	−0.001168	0.517510	−0.310523	0.069775
8.173000	0.001923	0.504471	−0.460511	0.108524
3.610318	−0.000887	0.091890	0.136389	−0.040169
1.697047	0.000382	−0.002315	0.729808	−0.223795
0.743532	−0.000148	0.002211	0.393480	−0.242889
0.158344	0.000054	−0.000470	0.015955	0.316665
0.075036	−0.000042	0.000370	−0.007576	0.571247
0.033091	0.000013	−0.000115	0.001945	0.266646

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−30.119890	−3.005962		−0.675116
12980.30	0.000082	−0.000030	159.5207	0.002236
3073.596	0.000729	−0.000267	47.59125	0.017550
998.1440	0.004154	−0.001523	17.77488	0.072061
381.4309	0.017788	−0.006602	7.342829	0.192108
161.3698	0.060010	−0.022649	3.166218	0.323334
73.26572	0.156617	−0.061485	1.344014	0.366212
34.84594	0.297784	−0.121851	0.544176	0.280379
17.08530	0.370383	−0.162513	0.199376	0.106208
8.520525	0.232558	−0.049058		
4.125417	0.049106	0.269386		
1.959216	0.001876	0.481602		
0.900822	0.000843	0.338381		
0.376944	−0.000004	0.065604		

Table CLV. Co ^4F $(21s13p10d)$ basis set. Energy(E_H) = −1381.414325

	s space			
Exponent	1s	2s	3s	4s
	−283.065400	−34.868280	−4.524237	−0.267396
8214702.	0.000004	−0.000001	0.000001	0.000000
1229997.	0.000033	−0.000010	0.000004	−0.000001
279909.8	0.000174	−0.000053	0.000020	−0.000004
79283.96	0.000736	−0.000225	0.000084	−0.000018
25865.95	0.002676	−0.000819	0.000305	−0.000064
9337.993	0.008666	−0.002663	0.000992	−0.000209
3641.978	0.025333	−0.007900	0.002955	−0.000623
1510.378	0.066450	−0.021334	0.007988	−0.001681
658.3879	0.151160	−0.051951	0.019674	−0.004153
298.9072	0.276818	−0.108746	0.041694	−0.008797
140.1820	0.348983	−0.180038	0.071928	−0.015302
66.86207	0.227427	−0.164539	0.068856	−0.014646
30.11571	0.042561	0.130560	−0.060654	0.012932
14.99109	−0.002395	0.548814	−0.354025	0.080652
7.395283	0.001725	0.430125	−0.408016	0.095851
3.311860	−0.000791	0.066554	0.227093	−0.063023
1.576977	0.000334	−0.001528	0.712754	−0.227351
0.708474	−0.000130	0.001717	0.346079	−0.225721
0.159535	0.000044	−0.000320	0.012662	0.327624
0.073281	−0.000033	0.000242	−0.005472	0.581972
0.032286	0.000010	−0.000076	0.001424	0.248876

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−30.120110	−3.006194		−0.675371
12975.47	0.000082	−0.000030	347.8080	0.000431
3072.467	0.000730	−0.000267	104.2943	0.003895
997.7808	0.004157	−0.001524	40.25363	0.019557
381.2931	0.017798	−0.006606	17.33864	0.064946
161.3129	0.060040	−0.022661	7.961278	0.157563
73.23915	0.156689	−0.061516	3.779184	0.265891
34.83113	0.297904	−0.121903	1.784861	0.322560
17.07665	0.370416	−0.162537	0.821742	0.293248
8.515381	0.232409	−0.048845	0.362061	0.181643
4.121952	0.049001	0.269815	0.146256	0.052202
1.957384	0.001864	0.481655		
0.900002	0.000843	0.337999		
0.376566	−0.000004	0.065411		

Table CLVI. Co ^4F $(21s14p8d)$ basis set. Energy(E_H) = −1381.413854

	s space			
Exponent	1s	2s	3s	4s
	−283.065300	−34.868060	−4.524008	−0.267317
8212419.	0.000004	−0.000001	0.000001	0.000000
1229662.	0.000033	−0.000010	0.000004	−0.000001
279834.4	0.000174	−0.000053	0.000020	−0.000004
79262.86	0.000737	−0.000225	0.000084	−0.000018
25859.22	0.002677	−0.000819	0.000305	−0.000064
9335.642	0.008669	−0.002664	0.000993	−0.000209
3641.092	0.025341	−0.007902	0.002956	−0.000623
1510.018	0.066467	−0.021340	0.007990	−0.001681
658.2343	0.151193	−0.051964	0.019679	−0.004154
298.8401	0.276854	−0.108766	0.041701	−0.008797
140.1524	0.348976	−0.180052	0.071935	−0.015301
66.84872	0.227368	−0.164502	0.068839	−0.014641
30.10868	0.042532	0.130707	−0.060724	0.012946
14.98768	−0.002395	0.548869	−0.354114	0.080662
7.393856	0.001724	0.429987	−0.407887	0.095808
3.311138	−0.000790	0.066512	0.227258	−0.063063
1.576794	0.000334	−0.001532	0.712653	−0.227286
0.708447	−0.000130	0.001718	0.346037	−0.225677
0.159627	0.000044	−0.000320	0.012657	0.326710
0.073357	−0.000033	0.000243	−0.005455	0.582337
0.032297	0.000010	−0.000076	0.001414	0.249390

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−30.119910	−3.005980		−0.675132
19267.78	0.000041	−0.000015	159.5896	0.002234
4560.986	0.000368	−0.000134	47.61216	0.017536
1481.436	0.002122	−0.000778	17.78333	0.072011
566.8671	0.009345	−0.003445	7.346457	0.192016
240.4910	0.033059	−0.012363	3.167773	0.323291
109.6105	0.094470	−0.036251	1.344597	0.366268
52.59491	0.208441	−0.083285	0.544351	0.280479
26.08361	0.332661	−0.139769	0.199402	0.106255
13.26143	0.331158	−0.142683		
6.799778	0.154915	0.035530		
3.393414	0.023488	0.338290		
1.648766	0.001418	0.461635		
0.776282	0.000401	0.270647		
0.325922	0.000047	0.041793		

Table CLVII. Co ^4F $(22s14p10d)$ basis set. Energy(E_H) = −1381.414429

	s space			
Exponent	1s	2s	3s	4s
	−283.065500	−34.868290	−4.524249	−0.267403
14371140.	0.000002	−0.000001	0.000000	0.000000
2151611.	0.000016	−0.000005	0.000002	0.000000
489604.9	0.000087	−0.000026	0.000010	−0.000002
138675.1	0.000366	−0.000112	0.000042	−0.000009
45243.56	0.001334	−0.000407	0.000152	−0.000032
16335.32	0.004344	−0.001332	0.000497	−0.000105
6372.265	0.012870	−0.003970	0.001480	−0.000311
2643.673	0.034802	−0.010946	0.004099	−0.000864
1153.506	0.084664	−0.027609	0.010356	−0.002179
524.8161	0.177586	−0.062877	0.023900	−0.005051
247.2875	0.295214	−0.121972	0.047058	−0.009928
119.8978	0.328179	−0.183131	0.073965	−0.015777
58.96049	0.182827	−0.132473	0.056001	−0.011876
27.13358	0.028281	0.196313	−0.094748	0.020331
13.68777	−0.001487	0.558238	−0.379970	0.087352
6.882110	0.001080	0.375137	−0.362448	0.084761
3.144470	−0.000499	0.052317	0.282440	−0.077154
1.506184	0.000187	−0.000548	0.698066	−0.228700
0.687253	−0.000078	0.001314	0.317708	−0.214872
0.160947	0.000025	−0.000208	0.011032	0.328424
0.072999	−0.000018	0.000155	−0.004459	0.587882
0.032064	0.000006	−0.000049	0.001153	0.244456

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−30.120130	−3.006207		−0.675381
19354.91	0.000041	−0.000015	347.7116	0.000431
4581.574	0.000365	−0.000133	104.2669	0.003897
1488.122	0.002106	−0.000772	40.24366	0.019565
569.4311	0.009276	−0.003419	17.33430	0.064971
241.5854	0.032830	−0.012276	7.958558	0.157650
110.1147	0.093889	−0.036020	3.777132	0.266035
52.84365	0.207449	−0.082868	1.783577	0.322608
26.21126	0.331867	−0.139365	0.821159	0.293122
13.32822	0.331839	−0.143150	0.361879	0.181494
6.835707	0.156418	0.033404	0.146205	0.052166
3.411006	0.023975	0.336507		
1.656920	0.001423	0.462283		
0.779779	0.000411	0.272588		
0.327409	0.000046	0.042401		

Table CLVIII. Co ^4F $(22s15p11d)$ basis set. Energy(E_H) = −1381.414484

	s space			
Exponent	1s	2s	3s	4s
	−283.065500	−34.868310	−4.524270	−0.267412
14370220.	0.000002	−0.000001	0.000000	0.000000
2151540.	0.000016	−0.000005	0.000002	0.000000
489625.7	0.000087	−0.000026	0.000010	−0.000002
138690.3	0.000366	−0.000112	0.000042	−0.000009
45249.89	0.001334	−0.000407	0.000152	−0.000032
16337.62	0.004343	−0.001331	0.000497	−0.000105
6373.073	0.012869	−0.003969	0.001480	−0.000311
2643.958	0.034798	−0.010945	0.004099	−0.000864
1153.614	0.084656	−0.027607	0.010355	−0.002179
524.8606	0.177574	−0.062872	0.023898	−0.005050
247.3069	0.295205	−0.121965	0.047056	−0.009928
119.9063	0.328188	−0.183128	0.073964	−0.015777
58.96429	0.182846	−0.132491	0.056008	−0.011878
27.13616	0.028288	0.196252	−0.094715	0.020324
13.68912	−0.001486	0.558217	−0.379934	0.087345
6.882771	0.001080	0.375202	−0.362501	0.084775
3.144647	−0.000499	0.052337	0.282368	−0.077137
1.506266	0.000187	−0.000551	0.698093	−0.228707
0.687268	−0.000078	0.001315	0.317737	−0.214889
0.160972	0.000025	−0.000208	0.011025	0.328299
0.073017	−0.000018	0.000155	−0.004451	0.587861
0.032071	0.000006	−0.000049	0.001152	0.244608

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−30.120150	−3.006228		−0.675402
28436.16	0.000021	−0.000008	502.1098	0.000195
6729.714	0.000187	−0.000068	151.0169	0.001825
2186.009	0.001088	−0.000398	58.57907	0.009942
837.0682	0.004887	−0.001796	25.65993	0.035933
355.8696	0.017907	−0.006646	11.96929	0.096910
162.6852	0.054417	−0.020558	5.836695	0.194129
78.48144	0.134187	−0.052408	2.883716	0.279852
39.30524	0.254367	−0.103408	1.407608	0.305933
20.17999	0.343659	−0.148307	0.670017	0.255925
10.55048	0.273619	−0.103049	0.305794	0.144761
5.501706	0.095826	0.122555	0.128703	0.036834
2.808052	0.010343	0.383827		
1.396517	0.001189	0.424845		
0.671372	0.000190	0.209207		
0.278964	0.000051	0.025487		

Table CLIX. Co ^4F $(23s15p11d)$ basis set. Energy(E_H) = −1381.414504

	s space			
Exponent	1s	2s	3s	4s
	−283.065500	−34.868320	−4.524273	−0.267412
24078730.	0.000001	0.000000	0.000000	0.000000
3605440.	0.000009	−0.000003	0.000001	0.000000
820548.8	0.000045	−0.000014	0.000005	−0.000001
232444.6	0.000192	−0.000059	0.000022	−0.000005
75845.92	0.000701	−0.000214	0.000080	−0.000017
27387.59	0.002287	−0.000699	0.000260	−0.000055
10685.00	0.006824	−0.002097	0.000783	−0.000165
4433.627	0.018769	−0.005821	0.002172	−0.000457
1935.129	0.047351	−0.015056	0.005645	−0.001191
881.1123	0.107218	−0.035701	0.013427	−0.002825
415.7653	0.207094	−0.076120	0.029059	−0.006148
202.2726	0.309588	−0.136503	0.053121	−0.011210
100.9430	0.297168	−0.181628	0.074297	−0.015902
51.08900	0.135911	−0.089616	0.038328	−0.008058
24.46336	0.016686	0.262315	−0.131612	0.028410
12.50342	−0.000270	0.556000	−0.400145	0.092820
6.397258	0.000394	0.321255	−0.311335	0.072183
2.992715	−0.000197	0.040547	0.330982	−0.089670
1.444009	0.000041	0.000315	0.681371	−0.229191
0.668411	−0.000026	0.000967	0.292856	−0.204889
0.162314	0.000007	−0.000117	0.009771	0.327791
0.072979	−0.000005	0.000087	−0.003714	0.592208
0.031967	0.000002	−0.000027	0.000953	0.242731

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−30.120160	−3.006230		−0.675403
28432.65	0.000021	−0.000008	502.1198	0.000195
6729.007	0.000187	−0.000068	151.0207	0.001825
2185.823	0.001088	−0.000399	58.58059	0.009942
837.0114	0.004888	−0.001796	25.66045	0.035932
355.8506	0.017908	−0.006646	11.96957	0.096906
162.6782	0.054420	−0.020559	5.836949	0.194117
78.47910	0.134188	−0.052408	2.883888	0.279844
39.30532	0.254352	−0.103402	1.407702	0.305931
20.18074	0.343643	−0.148298	0.670077	0.255927
10.55101	0.273631	−0.103062	0.305829	0.144778
5.501907	0.095839	0.122556	0.128716	0.036844
2.807868	0.010344	0.383906		
1.396290	0.001188	0.424855		
0.671247	0.000190	0.209133		
0.278920	0.000051	0.025471		

Table CLX. Co ^4F $(22s15p8d)$ basis set. Energy(E_H) = −1381.413922

	s space			
Exponent	1s	2s	3s	4s
	−283.065300	−34.868080	−4.524017	−0.267320
14369330.	0.000002	−0.000001	0.000000	0.000000
2151370.	0.000016	−0.000005	0.000002	0.000000
489582.1	0.000087	−0.000026	0.000010	−0.000002
138677.1	0.000366	−0.000112	0.000042	−0.000009
45245.40	0.001334	−0.000407	0.000152	−0.000032
16335.96	0.004343	−0.001331	0.000497	−0.000105
6372.410	0.012870	−0.003970	0.001480	−0.000311
2643.677	0.034802	−0.010946	0.004099	−0.000864
1153.488	0.084667	−0.027611	0.010356	−0.002179
524.8010	0.177593	−0.062880	0.023901	−0.005050
247.2778	0.295224	−0.121977	0.047060	−0.009927
119.8921	0.328179	−0.183135	0.073966	−0.015775
58.95739	0.182812	−0.132463	0.055996	−0.011874
27.13245	0.028275	0.196349	−0.094766	0.020333
13.68708	−0.001486	0.558244	−0.379984	0.087340
6.881899	0.001080	0.375101	−0.362409	0.084744
3.144460	−0.000499	0.052316	0.282416	−0.077147
1.506259	0.000187	−0.000549	0.698015	−0.228617
0.687307	−0.000078	0.001315	0.317769	−0.214881
0.161061	0.000025	−0.000208	0.011039	0.327375
0.073095	−0.000018	0.000155	−0.004452	0.588191
0.032084	0.000006	−0.000049	0.001148	0.245157

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−30.119920	−3.005988		−0.675138
28448.59	0.000021	−0.000008	159.5771	0.002234
6732.575	0.000187	−0.000068	47.60833	0.017539
2186.917	0.001087	−0.000398	17.78169	0.072022
837.4082	0.004884	−0.001795	7.345637	0.192042
356.0115	0.017895	−0.006641	3.167323	0.323320
162.7487	0.054387	−0.020547	1.344359	0.366275
78.51181	0.134127	−0.052382	0.544237	0.280450
39.31964	0.254311	−0.103385	0.199353	0.106213
20.18587	0.343700	−0.148311		
10.55198	0.273736	−0.103130		
5.500996	0.095852	0.122753		
2.805430	0.010326	0.384535		
1.394093	0.001183	0.424930		
0.669862	0.000190	0.208472		
0.278175	0.000051	0.025256		

Table CLXI. Co ^4F $(23s16p8d)$ basis set. Energy(E_H) = −1381.413951

	s space			
Exponent	1s	2s	3s	4s
	−283.065300	−34.868080	−4.524021	−0.267321
24075750.	0.000001	0.000000	0.000000	0.000000
3604823.	0.000009	−0.000003	0.000001	0.000000
820360.6	0.000045	−0.000014	0.000005	−0.000001
232379.2	0.000192	−0.000059	0.000022	−0.000005
75821.41	0.000701	−0.000214	0.000080	−0.000017
27377.73	0.002288	−0.000699	0.000261	−0.000055
10680.76	0.006827	−0.002098	0.000783	−0.000165
4431.716	0.018779	−0.005825	0.002173	−0.000457
1934.233	0.047378	−0.015064	0.005648	−0.001191
880.6771	0.107278	−0.035722	0.013435	−0.002826
415.5464	0.207191	−0.076163	0.029076	−0.006151
202.1596	0.309665	−0.136564	0.053147	−0.011213
100.8837	0.297095	−0.181640	0.074304	−0.015900
51.05853	0.135749	−0.089440	0.038255	−0.008042
24.45137	0.016642	0.262652	−0.131807	0.028450
12.49716	−0.000265	0.556018	−0.400279	0.092837
6.394316	0.000391	0.320942	−0.311019	0.072101
2.991815	−0.000196	0.040477	0.331264	−0.089743
1.443670	0.000040	0.000321	0.681223	−0.229104
0.668334	−0.000026	0.000965	0.292744	−0.204841
0.162450	0.000007	−0.000116	0.009772	0.326707
0.073073	−0.000005	0.000087	−0.003706	0.592608
0.031985	0.000002	−0.000027	0.000947	0.243393

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−30.119930	−3.005992		−0.675142
41961.40	0.000011	−0.000004	159.5563	0.002235
9928.306	0.000095	−0.000035	47.60204	0.017543
3224.971	0.000556	−0.000203	17.77925	0.072036
1235.293	0.002531	−0.000929	7.344608	0.192069
525.8469	0.009526	−0.003515	3.166851	0.323340
240.9762	0.030247	−0.011310	1.344142	0.366273
116.6418	0.080744	−0.030900	0.544144	0.280420
58.84834	0.174150	−0.069119	0.199319	0.106181
30.52910	0.287633	−0.119181		
16.16943	0.330064	−0.144454		
8.664236	0.212545	−0.050764		
4.591943	0.057802	0.195595		
2.381048	0.004967	0.406330		
1.206246	0.000899	0.382177		
0.588822	0.000137	0.160064		
0.239134	0.000034	0.015591		

Table CLXII. Co ^4F $(24s16p12d)$ basis set. Energy(E_H) = −1381.414532

	s space			
Exponent	1s	2s	3s	4s
	−283.065500	−34.868330	−4.524282	−0.267416
38211580.	0.000001	0.000000	0.000000	0.000000
5720364.	0.000005	−0.000002	0.000001	0.000000
1301533.	0.000026	−0.000008	0.000003	−0.000001
368629.4	0.000108	−0.000033	0.000012	−0.000003
120261.5	0.000394	−0.000120	0.000045	−0.000009
43418.24	0.001289	−0.000394	0.000147	−0.000031
16936.40	0.003863	−0.001183	0.000441	−0.000093
7026.505	0.010723	−0.003307	0.001235	−0.000260
3066.441	0.027621	−0.008640	0.003228	−0.000679
1396.209	0.065263	−0.021068	0.007909	−0.001669
658.9394	0.137290	−0.047103	0.017790	−0.003743
320.5720	0.241935	−0.093698	0.035975	−0.007622
160.0213	0.317901	−0.153781	0.060635	−0.012804
81.43815	0.251862	−0.171878	0.071470	−0.015370
41.75655	0.084599	−0.021860	0.009314	−0.001764
21.19516	0.006265	0.344462	−0.183372	0.039922
11.06466	0.000879	0.533966	−0.415523	0.097565
5.781467	−0.000236	0.252844	−0.234585	0.053018
2.793499	0.000070	0.027913	0.388419	−0.104703
1.366512	−0.000081	0.001089	0.654712	−0.228639
0.644773	0.000018	0.000627	0.262271	−0.191803
0.163977	−0.000007	−0.000035	0.008397	0.326376
0.073105	0.000005	0.000029	−0.002953	0.596412
0.031929	−0.000001	−0.000009	0.000749	0.242269

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−30.120170	−3.006238		−0.675411
40907.90	0.000011	−0.000004	725.5543	0.000088
9685.545	0.000099	−0.000036	218.5446	0.000843
3148.973	0.000578	−0.000212	84.83172	0.004886
1207.509	0.002628	−0.000964	37.51021	0.019319
514.5579	0.009858	−0.003638	17.75380	0.056346
236.0120	0.031186	−0.011667	8.790153	0.129030
114.3264	0.082860	−0.031737	4.475086	0.220265
57.71241	0.177538	−0.070547	2.280777	0.282363
29.94897	0.290705	−0.120644	1.145275	0.284992
15.86664	0.329017	−0.144039	0.561196	0.222026
8.500474	0.207313	−0.045024	0.264108	0.115844
4.499628	0.054586	0.204111	0.115192	0.026385
2.332717	0.004523	0.408983		
1.182999	0.000876	0.376388		
0.578196	0.000127	0.153878		
0.233600	0.000032	0.014497		

Table CLXIII. Ni ^3F ($19s13p8d$) basis set. Energy(E_H) = −1506.869768

	s space			
Exponent	1s	2s	3s	4s
	−305.618600	−37.917370	−4.887376	−0.276014
4982136.	0.000009	−0.000003	0.000001	0.000000
746055.0	0.000068	−0.000021	0.000008	−0.000002
169781.6	0.000357	−0.000109	0.000041	−0.000008
48088.72	0.001505	−0.000462	0.000173	−0.000036
15687.42	0.005449	−0.001678	0.000629	−0.000130
5662.562	0.017475	−0.005434	0.002041	−0.000424
2207.835	0.049883	−0.015887	0.005973	−0.001233
914.9032	0.123838	−0.041616	0.015785	−0.003284
398.0467	0.250644	−0.094574	0.036276	−0.007494
180.0034	0.359297	−0.171917	0.068295	−0.014339
83.40268	0.276003	−0.192516	0.080260	−0.016595
37.66537	0.065402	0.052743	−0.023325	0.004271
18.17357	−0.001613	0.526633	−0.322403	0.072742
8.733607	0.001957	0.494931	−0.456371	0.103078
3.850966	−0.000878	0.086166	0.165601	−0.041289
1.801338	0.000354	−0.001860	0.733815	−0.234932
0.783408	−0.000120	0.001835	0.372876	−0.216238
0.133283	0.000022	−0.000176	0.008708	0.594640
0.046685	−0.000009	0.000075	−0.002456	0.549389

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−32.941290	−3.277243		−0.706470
14093.07	0.000082	−0.000030	174.0680	0.002280
3337.066	0.000724	−0.000267	51.96332	0.017974
1083.716	0.004130	−0.001527	19.43926	0.074036
414.1688	0.017709	−0.006628	8.046696	0.196017
175.2636	0.059858	−0.022787	3.470439	0.325762
79.60635	0.156580	−0.062024	1.470409	0.364142
37.88973	0.298300	−0.123306	0.592561	0.277037
18.59944	0.370562	−0.163994	0.215508	0.105906
9.285933	0.231680	−0.047148		
4.502064	0.048810	0.273189		
2.139442	0.001974	0.481351		
0.983353	0.000863	0.335319		
0.411062	0.000011	0.064882		

Table CLXIV. Ni ^3F $(20s12p8d)$ basis set. Energy(E_H) = −1506.869674

	s space			
Exponent	1s	2s	3s	4s
	−305.618700	−37.917450	−4.887452	−0.276104
5049037.	0.000009	−0.000003	0.000001	0.000000
756070.6	0.000067	−0.000020	0.000008	−0.000002
172060.7	0.000351	−0.000108	0.000040	−0.000008
48734.27	0.001480	−0.000454	0.000170	−0.000035
15898.03	0.005360	−0.001651	0.000618	−0.000128
5738.594	0.017194	−0.005345	0.002008	−0.000416
2237.487	0.049116	−0.015638	0.005878	−0.001218
927.2095	0.122143	−0.040990	0.015545	−0.003224
403.4238	0.248073	−0.093376	0.035804	−0.007434
182.4631	0.358249	−0.170379	0.067635	−0.014114
84.60570	0.279148	−0.193759	0.080670	−0.016916
38.43278	0.068341	0.043423	−0.018893	0.003920
18.47292	−0.001177	0.519382	−0.315297	0.069758
8.870270	0.001913	0.503849	−0.461267	0.106885
3.920309	−0.000881	0.091450	0.144745	−0.041576
1.840423	0.000377	−0.002236	0.730175	−0.221085
0.804856	−0.000145	0.002180	0.388310	−0.235758
0.169869	0.000051	−0.000450	0.015474	0.314058
0.079435	−0.000040	0.000352	−0.007303	0.570786
0.034712	0.000012	−0.000110	0.001894	0.267696

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−32.941350	−3.277308		−0.706544
9161.715	0.000173	−0.000064	174.0203	0.002282
2170.238	0.001523	−0.000562	51.94890	0.017983
704.3862	0.008501	−0.003162	19.43315	0.074072
268.5188	0.035057	−0.013189	8.043555	0.196110
113.1712	0.110039	−0.042788	3.468674	0.325859
50.98755	0.251357	−0.101824	1.469527	0.364133
23.91277	0.382316	−0.165831	0.592174	0.276926
11.50698	0.309371	−0.114481	0.215408	0.105792
5.446953	0.087507	0.188737		
2.538589	0.004120	0.481531		
1.137292	0.001343	0.402750		
0.468668	−0.000037	0.095638		

Table CLXV. Ni ^3F $(20s13p8d)$ basis set. Energy(E_H) = −1506.869853

	s space			
Exponent	1s	2s	3s	4s
	−305.618700	−37.917470	−4.887467	−0.276116
5047045.	0.000009	−0.000003	0.000001	0.000000
755772.8	0.000067	−0.000020	0.000008	−0.000002
171992.9	0.000351	−0.000108	0.000040	−0.000008
48715.07	0.001481	−0.000454	0.000170	−0.000035
15891.77	0.005363	−0.001652	0.000619	−0.000128
5736.339	0.017202	−0.005348	0.002008	−0.000416
2236.614	0.049139	−0.015645	0.005881	−0.001218
926.8451	0.122193	−0.041008	0.015552	−0.003226
403.2611	0.248153	−0.093413	0.035818	−0.007437
182.3871	0.358286	−0.170428	0.067657	−0.014119
84.56789	0.279054	−0.193724	0.080657	−0.016913
38.40807	0.068248	0.043714	−0.019025	0.003946
18.46340	−0.001193	0.519615	−0.315535	0.069820
8.865952	0.001916	0.503572	−0.461087	0.106841
3.917881	−0.000882	0.091291	0.145320	−0.041712
1.839535	0.000378	−0.002242	0.730087	−0.221136
0.804595	−0.000145	0.002179	0.387996	−0.235634
0.169850	0.000051	−0.000449	0.015431	0.314294
0.079399	−0.000040	0.000352	−0.007264	0.570894
0.034698	0.000012	−0.000110	0.001884	0.267372

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−32.941390	−3.277331		−0.706560
14096.01	0.000082	−0.000030	174.0626	0.002281
3337.761	0.000724	−0.000267	51.96169	0.017975
1083.942	0.004128	−0.001526	19.43859	0.074039
414.2554	0.017703	−0.006626	8.046377	0.196025
175.3005	0.059839	−0.022780	3.470270	0.325768
79.62322	0.156541	−0.062008	1.470338	0.364137
37.89802	0.298250	−0.123283	0.592502	0.277047
18.60373	0.370561	−0.163991	0.215479	0.105889
9.288240	0.231752	−0.047234		
4.503387	0.048850	0.273044		
2.140122	0.001977	0.481342		
0.983685	0.000863	0.335418		
0.411269	0.000011	0.064974		

Table CLXVI. Ni ^3F $(20s12p9d)$ basis set. Energy(E_H) = −1506.870211

	s space			
Exponent	1s	2s	3s	4s
	−305.618800	−37.917660	−4.887676	−0.276184
5048010.	0.000009	−0.000003	0.000001	0.000000
755918.1	0.000067	−0.000020	0.000008	−0.000002
172026.2	0.000351	−0.000108	0.000040	−0.000008
48724.57	0.001480	−0.000454	0.000170	−0.000035
15894.89	0.005361	−0.001651	0.000619	−0.000128
5737.468	0.017198	−0.005346	0.002008	−0.000416
2237.051	0.049128	−0.015641	0.005880	−0.001218
927.0302	0.122167	−0.040999	0.015548	−0.003226
403.3461	0.248109	−0.093393	0.035810	−0.007436
182.4282	0.358262	−0.170400	0.067645	−0.014118
84.58917	0.279103	−0.193742	0.080663	−0.016917
38.42293	0.068300	0.043544	−0.018947	0.003931
18.46879	−0.001182	0.519495	−0.315412	0.069796
8.868190	0.001914	0.503738	−0.461196	0.106880
3.918870	−0.000881	0.091368	0.145071	−0.041660
1.839853	0.000378	−0.002243	0.730174	−0.221161
0.804663	−0.000145	0.002180	0.388081	−0.235718
0.169846	0.000051	−0.000449	0.015442	0.314679
0.079370	−0.000040	0.000352	−0.007285	0.570730
0.034700	0.000012	−0.000110	0.001893	0.267189

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−32.941550	−3.277520		−0.706780
9148.796	0.000174	−0.000064	258.8667	0.000993
2167.171	0.001527	−0.000563	77.49604	0.008509
703.3857	0.008521	−0.003169	29.58972	0.038870
268.1342	0.035135	−0.013218	12.51527	0.117795
113.0078	0.110247	−0.042873	5.624468	0.241115
50.91339	0.251691	−0.101966	2.551303	0.331340
23.87740	0.382481	−0.165937	1.128060	0.328066
11.48924	0.308988	−0.114099	0.475373	0.223691
5.436884	0.087135	0.189657	0.182128	0.074072
2.533837	0.004066	0.481780		
1.135309	0.001344	0.402020		
0.467891	−0.000039	0.095189		

Table CLXVII. Ni ^3F $(20s13p9d)$ basis set. Energy(E_H) = −1506.870391

	s space			
Exponent	1s	2s	3s	4s
	−305.618800	−37.917680	−4.887692	−0.276196
5045991.	0.000009	−0.000003	0.000001	0.000000
755614.2	0.000067	−0.000020	0.000008	−0.000002
171956.8	0.000351	−0.000108	0.000040	−0.000008
48704.79	0.001481	−0.000454	0.000170	−0.000035
15888.41	0.005364	−0.001652	0.000619	−0.000128
5735.123	0.017207	−0.005349	0.002009	−0.000416
2236.137	0.049151	−0.015649	0.005883	−0.001219
926.6468	0.122220	−0.041018	0.015556	−0.003227
403.1743	0.248194	−0.093432	0.035825	−0.007440
182.3476	0.358302	−0.170452	0.067668	−0.014124
84.54885	0.279004	−0.193705	0.080649	−0.016914
38.39634	0.068201	0.043856	−0.019089	0.003959
18.45859	−0.001199	0.519744	−0.315667	0.069863
8.863548	0.001917	0.503442	−0.461004	0.106833
3.916227	−0.000883	0.091196	0.145697	−0.041806
1.838870	0.000378	−0.002249	0.730089	−0.221223
0.804362	−0.000145	0.002178	0.387729	−0.235576
0.169797	0.000051	−0.000449	0.015392	0.315120
0.079306	−0.000040	0.000351	−0.007243	0.570851
0.034677	0.000012	−0.000110	0.001883	0.266650

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−32.941590	−3.277544		−0.706796
14106.62	0.000082	−0.000030	258.7090	0.000994
3340.269	0.000723	−0.000267	77.44880	0.008519
1084.756	0.004123	−0.001524	29.57058	0.038911
414.5683	0.017681	−0.006618	12.50603	0.117917
175.4340	0.059774	−0.022755	5.619606	0.241288
79.68282	0.156411	−0.061955	2.548927	0.331378
37.92578	0.298105	−0.123216	1.127141	0.327908
18.61690	0.370597	−0.164007	0.475122	0.223513
9.294179	0.231993	−0.047454	0.182060	0.074029
4.505399	0.048942	0.272913		
2.140633	0.001975	0.481490		
0.983698	0.000865	0.335509		
0.411177	0.000010	0.064942		

Table CLXVIII. Ni ^3F $(21s13p10d)$ basis set. Energy(E_H) = −1506.870653

	s space			
Exponent	1s	2s	3s	4s
	−305.619000	−37.917770	−4.887776	−0.276223
8865538.	0.000004	−0.000001	0.000001	0.000000
1327434.	0.000033	−0.000010	0.000004	−0.000001
302079.4	0.000174	−0.000053	0.000020	−0.000004
85562.28	0.000734	−0.000225	0.000084	−0.000017
27913.89	0.002666	−0.000819	0.000307	−0.000064
10077.23	0.008635	−0.002666	0.000999	−0.000207
3930.268	0.025245	−0.007909	0.002974	−0.000617
1629.935	0.066240	−0.021367	0.008042	−0.001665
710.5214	0.150781	−0.052069	0.019824	−0.004118
322.6014	0.276418	−0.109123	0.042071	−0.008734
151.3200	0.349065	−0.180932	0.072709	−0.015221
72.20548	0.228094	−0.165716	0.069821	−0.014614
32.56308	0.042831	0.131488	−0.061771	0.012966
16.24010	−0.002436	0.550620	−0.359311	0.080591
8.021107	0.001722	0.428700	−0.406872	0.093978
3.596586	−0.000786	0.066086	0.235545	−0.064138
1.709939	0.000331	−0.001418	0.712116	−0.224325
0.766710	−0.000127	0.001679	0.341235	−0.218837
0.171131	0.000042	−0.000302	0.012288	0.324209
0.077694	−0.000031	0.000228	−0.005272	0.581003
0.033917	0.000010	−0.000072	0.001382	0.251073

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−32.941670	−3.277619		−0.706876
14091.36	0.000082	−0.000030	378.5519	0.000441
3336.647	0.000724	−0.000268	113.5686	0.003995
1083.577	0.004130	−0.001527	43.85692	0.020128
414.1156	0.017712	−0.006629	18.91472	0.066988
175.2423	0.059867	−0.022791	8.698675	0.161435
79.59560	0.156612	−0.062039	4.130155	0.269063
37.88229	0.298371	−0.123336	1.948298	0.322048
18.59440	0.370595	−0.164017	0.894255	0.289694
9.282603	0.231605	−0.047015	0.392075	0.179215
4.499480	0.048745	0.273494	0.157317	0.052077
2.138001	0.001964	0.481411		
0.982705	0.000863	0.335014		
0.410805	0.000011	0.064761		

Table CLXIX. Ni ^3F ($21s14p10d$) basis set. Energy(E_H) = −1506.870716

	s space			
Exponent	1s	2s	3s	4s
	−305.619000	−37.917780	−4.887784	−0.276229
8861571.	0.000004	−0.000001	0.000001	0.000000
1326856.	0.000033	−0.000010	0.000004	−0.000001
301951.9	0.000174	−0.000053	0.000020	−0.000004
85527.34	0.000734	−0.000225	0.000084	−0.000017
27902.88	0.002667	−0.000820	0.000308	−0.000064
10073.40	0.008638	−0.002667	0.000999	−0.000207
3928.823	0.025256	−0.007913	0.002976	−0.000617
1629.348	0.066266	−0.021375	0.008045	−0.001666
710.2698	0.150831	−0.052089	0.019832	−0.004120
322.4904	0.276475	−0.109154	0.042083	−0.008736
151.2699	0.349057	−0.180959	0.072722	−0.015225
72.18211	0.228002	−0.165654	0.069795	−0.014608
32.54910	0.042783	0.131744	−0.061897	0.012992
16.23357	−0.002439	0.550726	−0.359473	0.080634
8.018163	0.001722	0.428459	−0.406664	0.093926
3.595066	−0.000786	0.065997	0.235941	−0.064234
1.709326	0.000331	−0.001419	0.712029	−0.224356
0.766505	−0.000127	0.001678	0.341006	−0.218744
0.171125	0.000042	−0.000302	0.012257	0.324354
0.077668	−0.000031	0.000228	−0.005248	0.581129
0.033905	0.000010	−0.000072	0.001375	0.250821

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−32.941680	−3.277630		−0.706884
21027.92	0.000041	−0.000015	378.4588	0.000441
4977.560	0.000362	−0.000133	113.5420	0.003997
1616.740	0.002090	−0.000773	43.84726	0.020135
618.6718	0.009218	−0.003427	18.91037	0.067013
262.5183	0.032683	−0.012324	8.695874	0.161517
119.6907	0.093673	−0.036254	4.128081	0.269192
57.46585	0.207510	−0.083667	1.947009	0.322090
28.52829	0.332410	−0.141044	0.893662	0.289579
14.52148	0.331687	−0.143811	0.391894	0.179077
7.453850	0.155755	0.036243	0.157269	0.052048
3.723553	0.023873	0.339498		
1.809813	0.001499	0.460930		
0.851336	0.000432	0.269963		
0.357241	0.000056	0.042013		

Table CLXX. Ni ^3F ($21s14p8d$) basis set. Energy(E_H) = -1506.870031

	s space			
Exponent	1s	2s	3s	4s
	−305.618700	−37.917500	−4.887488	−0.276123
8862958.	0.000004	−0.000001	0.000001	0.000000
1327061.	0.000033	−0.000010	0.000004	−0.000001
301997.2	0.000174	−0.000053	0.000020	−0.000004
85539.75	0.000734	−0.000225	0.000084	−0.000017
27906.79	0.002667	−0.000820	0.000307	−0.000064
10074.78	0.008637	−0.002666	0.000999	−0.000207
3929.346	0.025252	−0.007911	0.002975	−0.000617
1629.561	0.066257	−0.021372	0.008044	−0.001665
710.3610	0.150813	−0.052081	0.019829	−0.004118
322.5312	0.276453	−0.109143	0.042078	−0.008734
151.2889	0.349058	−0.180948	0.072716	−0.015220
72.19107	0.228038	−0.165678	0.069804	−0.014608
32.55376	0.042802	0.131657	−0.061854	0.012982
16.23585	−0.002439	0.550679	−0.359407	0.080600
8.019377	0.001723	0.428537	−0.406728	0.093930
3.595920	−0.000787	0.066041	0.235702	−0.064172
1.709769	0.000331	−0.001418	0.712013	−0.224251
0.766692	−0.000127	0.001679	0.341207	−0.218788
0.171221	0.000042	−0.000303	0.012288	0.323277
0.077779	−0.000031	0.000228	−0.005259	0.581320
0.033930	0.000010	−0.000072	0.001373	0.251644

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−32.941410	−3.277350		−0.706576
20921.27	0.000041	−0.000015	174.1315	0.002279
4952.300	0.000365	−0.000135	51.98277	0.017962
1608.526	0.002109	−0.000780	19.44713	0.073991
615.5190	0.009297	−0.003456	8.050054	0.195940
261.1717	0.032942	−0.012423	3.471843	0.325730
119.0709	0.094330	−0.036517	1.470927	0.364191
57.16096	0.208630	−0.084143	0.592679	0.277137
28.37169	0.333318	−0.141510	0.215505	0.105932
14.43889	0.330927	−0.143267		
7.408909	0.154048	0.038726		
3.701089	0.023314	0.341600		
1.799313	0.001491	0.460126		
0.846871	0.000420	0.267682		
0.355382	0.000057	0.041320		

Table CLXXI. Ni ^3F $(22s14p10d)$ basis set. Energy(E_H) = −1506.870765

	s space			
Exponent	1s	2s	3s	4s
	−305.619000	−37.917780	−4.887789	−0.276229
15500640.	0.000002	−0.000001	0.000000	0.000000
2320782.	0.000016	−0.000005	0.000002	0.000000
528142.4	0.000086	−0.000026	0.000010	−0.000002
149601.5	0.000365	−0.000112	0.000042	−0.000009
48809.94	0.001330	−0.000408	0.000153	−0.000032
17622.95	0.004329	−0.001333	0.000500	−0.000104
6874.435	0.012829	−0.003976	0.001490	−0.000308
2851.945	0.034698	−0.010965	0.004127	−0.000856
1244.364	0.084446	−0.027670	0.010434	−0.002160
566.1636	0.177251	−0.063065	0.024099	−0.005011
266.7899	0.294960	−0.122481	0.047523	−0.009866
129.3762	0.328392	−0.184140	0.074815	−0.015704
63.65175	0.183342	−0.133380	0.056796	−0.011853
29.33068	0.028413	0.198117	−0.096757	0.020445
14.82094	−0.001519	0.559788	−0.385380	0.087218
7.459898	0.001076	0.373223	−0.359869	0.082725
3.413332	−0.000495	0.051819	0.290900	−0.078085
1.632793	0.000185	−0.000450	0.696741	−0.225454
0.743569	−0.000076	0.001280	0.313029	−0.208130
0.172599	0.000024	−0.000194	0.010711	0.324923
0.077425	−0.000017	0.000144	−0.004302	0.586522
0.033701	0.000005	−0.000046	0.001120	0.247028

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−32.941690	−3.277633		−0.706887
21027.22	0.000041	−0.000015	378.4560	0.000441
4977.395	0.000362	−0.000133	113.5405	0.003997
1616.690	0.002091	−0.000773	43.84651	0.020136
618.6550	0.009219	−0.003427	18.91010	0.067014
262.5125	0.032684	−0.012325	8.695728	0.161522
119.6897	0.093672	−0.036253	4.127933	0.269204
57.46650	0.207503	−0.083664	1.946910	0.322092
28.52865	0.332416	−0.141046	0.893621	0.289571
14.52125	0.331703	−0.143820	0.391876	0.179070
7.453395	0.155749	0.036277	0.157261	0.052041
3.723037	0.023864	0.339571		
1.809540	0.001498	0.460898		
0.851260	0.000432	0.269899		
0.357237	0.000056	0.042008		

Table CLXXII. Ni ^3F $(22s15p11d)$ basis set. Energy(E_H) = −1506.870831

	s space			
Exponent	1s	2s	3s	4s
	−305.619000	−37.917810	−4.887814	−0.276241
15503020.	0.000002	−0.000001	0.000000	0.000000
2321071.	0.000016	−0.000005	0.000002	0.000000
528180.2	0.000086	−0.000026	0.000010	−0.000002
149604.0	0.000365	−0.000112	0.000042	−0.000009
48809.07	0.001330	−0.000408	0.000153	−0.000032
17622.39	0.004330	−0.001333	0.000500	−0.000104
6874.201	0.012830	−0.003976	0.001490	−0.000308
2851.857	0.034699	−0.010965	0.004128	−0.000856
1244.334	0.084447	−0.027670	0.010434	−0.002160
566.1547	0.177252	−0.063065	0.024100	−0.005012
266.7873	0.294960	−0.122482	0.047524	−0.009866
129.3752	0.328391	−0.184139	0.074814	−0.015704
63.65161	0.183337	−0.133383	0.056798	−0.011854
29.33302	0.028413	0.198072	−0.096733	0.020440
14.82212	−0.001516	0.559769	−0.385348	0.087212
7.460513	0.001074	0.373274	−0.359917	0.082737
3.413576	−0.000495	0.051836	0.290828	−0.078065
1.632884	0.000185	−0.000452	0.696778	−0.225470
0.743579	−0.000076	0.001281	0.313056	−0.208139
0.172592	0.000024	−0.000195	0.010703	0.324987
0.077420	−0.000017	0.000144	−0.004295	0.586481
0.033701	0.000005	−0.000046	0.001119	0.247009

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−32.941710	−3.277659		−0.706912
30915.05	0.000021	−0.000008	545.8386	0.000200
7316.099	0.000185	−0.000068	164.2348	0.001875
2376.414	0.001079	−0.000398	63.73401	0.010238
909.9714	0.004849	−0.001797	27.93862	0.037119
386.8928	0.017795	−0.006660	13.05187	0.099934
176.9042	0.054185	−0.020646	6.370591	0.198144
85.36992	0.133943	−0.052781	3.146446	0.281918
42.78105	0.254546	−0.104497	1.533327	0.304188
21.98602	0.344043	−0.149923	0.727428	0.252258
11.50565	0.273283	−0.102684	0.330410	0.142773
6.004377	0.095480	0.125776	0.138179	0.036753
3.066800	0.010373	0.385796		
1.525658	0.001240	0.422726		
0.733092	0.000211	0.207155		
0.304634	0.000058	0.025317		

Table CLXXIII. Ni ^3F $(23s15p11d)$ basis set. Energy(E_H) = −1506.870853

	s space			
Exponent	1s	2s	3s	4s
	−305.619000	−37.917810	−4.887817	−0.276241
26074180.	0.000001	0.000000	0.000000	0.000000
3900623.	0.000009	−0.000003	0.000001	0.000000
887188.9	0.000045	−0.000014	0.000005	−0.000001
251219.4	0.000191	−0.000059	0.000022	−0.000005
81947.81	0.000697	−0.000214	0.000080	−0.000017
29584.06	0.002277	−0.000699	0.000262	−0.000054
11539.64	0.006794	−0.002098	0.000787	−0.000163
4787.417	0.018693	−0.005825	0.002185	−0.000452
2089.223	0.047180	−0.015072	0.005680	−0.001179
951.1524	0.106906	−0.035765	0.013523	−0.002799
448.7763	0.206700	−0.076344	0.029301	−0.006100
218.3280	0.309432	−0.137099	0.053662	−0.011142
108.9656	0.297599	−0.182728	0.075195	−0.015838
55.17298	0.136436	−0.090289	0.038925	−0.008053
26.45048	0.016765	0.264633	−0.134412	0.028574
13.53761	−0.000297	0.557127	−0.405305	0.092544
6.932072	0.000391	0.319202	−0.307555	0.070060
3.247388	−0.000196	0.040089	0.339154	−0.090368
1.565164	0.000041	0.000390	0.679442	−0.225746
0.723071	−0.000025	0.000940	0.288396	−0.198304
0.173996	0.000007	−0.000107	0.009490	0.324397
0.077406	−0.000005	0.000080	−0.003588	0.590494
0.033608	0.000002	−0.000025	0.000927	0.245455

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−32.941720	−3.277660		−0.706914
30916.64	0.000021	−0.000008	545.9420	0.000200
7316.740	0.000185	−0.000068	164.2648	0.001875
2376.699	0.001078	−0.000398	63.74461	0.010235
910.1014	0.004848	−0.001797	27.94271	0.037112
386.9528	0.017790	−0.006658	13.05354	0.099920
176.9320	0.054173	−0.020641	6.371350	0.198129
85.38351	0.133916	−0.052769	3.146767	0.281921
42.78871	0.254501	−0.104477	1.533438	0.304202
21.99048	0.344023	−0.149910	0.727470	0.252267
11.50805	0.273336	−0.102732	0.330426	0.142783
6.005561	0.095530	0.125706	0.138183	0.036757
3.067107	0.010381	0.385834		
1.525658	0.001240	0.422771		
0.733065	0.000211	0.207141		
0.304630	0.000058	0.025315		

Table CLXXIV. Ni ^3F $(23s16p10d)$ basis set. Energy(E_H) = −1506.870820

	s space			
Exponent	1s	2s	3s	4s
	−305.619000	−37.917790	−4.887797	−0.276234
25983870.	0.000001	0.000000	0.000000	0.000000
3890234.	0.000009	−0.000003	0.000001	0.000000
885337.5	0.000045	−0.000014	0.000005	−0.000001
250791.2	0.000191	−0.000059	0.000022	−0.000005
81827.53	0.000698	−0.000214	0.000080	−0.000017
29545.20	0.002280	−0.000700	0.000262	−0.000054
11525.81	0.006803	−0.002100	0.000788	−0.000163
4782.133	0.018716	−0.005832	0.002187	−0.000453
2087.097	0.047230	−0.015088	0.005686	−0.001180
950.2591	0.107000	−0.035800	0.013537	−0.002802
448.3854	0.206829	−0.076403	0.029324	−0.006105
218.1483	0.309510	−0.137177	0.053695	−0.011149
108.8779	0.297486	−0.182727	0.075199	−0.015838
55.12909	0.136212	−0.090082	0.038838	−0.008035
26.44114	0.016704	0.264878	−0.134556	0.028605
13.53319	−0.000282	0.557107	−0.405367	0.092559
6.930146	0.000384	0.319006	−0.307365	0.070015
3.246905	−0.000192	0.040048	0.339315	−0.090412
1.564926	0.000039	0.000394	0.679402	−0.225746
0.722978	−0.000025	0.000939	0.288299	−0.198276
0.174043	0.000007	−0.000107	0.009480	0.324204
0.077422	−0.000005	0.000080	−0.003579	0.590632
0.033611	0.000001	−0.000025	0.000925	0.245523

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−32.941700	−3.277641		−0.706893
45066.62	0.000011	−0.000004	378.3807	0.000442
10662.64	0.000096	−0.000035	113.5157	0.003999
3463.431	0.000563	−0.000207	43.83571	0.020145
1326.624	0.002563	−0.000948	18.90485	0.067042
564.7414	0.009650	−0.003591	8.693255	0.161564
258.8288	0.030653	−0.011562	4.126972	0.269198
125.3115	0.081822	−0.031602	1.946709	0.322023
63.24233	0.176293	−0.070668	0.893687	0.289515
32.82406	0.290245	−0.121616	0.391957	0.179094
17.39692	0.329778	−0.145531	0.157273	0.052069
9.324394	0.208547	−0.045304		
4.938839	0.055274	0.205169		
2.562025	0.004691	0.409133		
1.299294	0.000923	0.375322		
0.634678	0.000147	0.154078		
0.257086	0.000037	0.014745		

Table CLXXV. Ni ^3F $(23s16p12d)$ basis set. Energy(E_H) = −1506.870874

	s space			
Exponent	1s	2s	3s	4s
	−305.619000	−37.917820	−4.887826	−0.276245
26141900.	0.000001	0.000000	0.000000	0.000000
3910302.	0.000009	−0.000003	0.000001	0.000000
889408.3	0.000045	−0.000014	0.000005	−0.000001
251842.6	0.000191	−0.000058	0.000022	−0.000005
82142.06	0.000695	−0.000213	0.000080	−0.000017
29649.63	0.002271	−0.000697	0.000261	−0.000054
11563.35	0.006778	−0.002093	0.000785	−0.000163
4796.523	0.018653	−0.005812	0.002180	−0.000451
2092.909	0.047092	−0.015042	0.005669	−0.001177
952.7051	0.106744	−0.035706	0.013501	−0.002795
449.4476	0.206491	−0.076245	0.029263	−0.006092
218.6193	0.309358	−0.137007	0.053622	−0.011134
109.0891	0.297858	−0.182759	0.075204	−0.015839
55.22226	0.136717	−0.090644	0.039070	−0.008085
26.47918	0.016816	0.263964	−0.134004	0.028485
13.55131	−0.000287	0.557128	−0.405081	0.092484
6.938454	0.000387	0.319832	−0.308125	0.070201
3.248523	−0.000194	0.040232	0.338696	−0.090260
1.565752	0.000040	0.000364	0.679571	−0.225724
0.723272	−0.000025	0.000949	0.288620	−0.198412
0.174063	0.000007	−0.000109	0.009502	0.323969
0.077469	−0.000005	0.000082	−0.003592	0.590404
0.033633	0.000002	−0.000026	0.000928	0.245963

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−32.941730	−3.277669		−0.706923
45479.84	0.000011	−0.000004	775.3778	0.000093
10752.52	0.000095	−0.000035	234.1655	0.000891
3490.414	0.000555	−0.000205	91.12659	0.005141
1336.281	0.002533	−0.000937	40.37520	0.020267
568.6093	0.009547	−0.003552	19.14970	0.058975
260.5021	0.030367	−0.011453	9.503048	0.133708
126.0747	0.081200	−0.031354	4.842981	0.224600
63.60369	0.175362	−0.070272	2.467929	0.283188
32.99937	0.289526	−0.121259	1.237743	0.281639
17.48273	0.330243	−0.145738	0.604980	0.217485
9.367328	0.209946	−0.046736	0.283697	0.113473
4.960836	0.056013	0.203413	0.123139	0.026097
2.572762	0.004779	0.408790		
1.304166	0.000929	0.376563		
0.636775	0.000148	0.155224		
0.258084	0.000038	0.014930		

Table CLXXVI. Ni ^3F $(23s16p8d)$ basis set. Energy(E_H) = −1506.870135

	s space			
Exponent	1s	2s	3s	4s
	−305.618800	−37.917510	−4.887502	−0.276128
26004250.	0.000001	0.000000	0.000000	0.000000
3891914.	0.000009	−0.000003	0.000001	0.000000
885564.9	0.000045	−0.000014	0.000005	−0.000001
250828.3	0.000191	−0.000059	0.000022	−0.000005
81833.52	0.000698	−0.000214	0.000080	−0.000017
29544.88	0.002280	−0.000700	0.000262	−0.000054
11524.40	0.006805	−0.002101	0.000788	−0.000163
4780.975	0.018724	−0.005835	0.002188	−0.000453
2086.362	0.047256	−0.015097	0.005689	−0.001181
949.8329	0.107062	−0.035822	0.013545	−0.002803
448.1485	0.206938	−0.076451	0.029343	−0.006108
218.0194	0.309600	−0.137244	0.053723	−0.011153
108.8093	0.297406	−0.182744	0.075209	−0.015838
55.09427	0.136041	−0.089874	0.038751	−0.008015
26.42284	0.016659	0.265352	−0.134832	0.028661
13.52346	−0.000281	0.557142	−0.405575	0.092595
6.925407	0.000383	0.318559	−0.306878	0.069885
3.245022	−0.000192	0.039943	0.339823	−0.090531
1.564204	0.000039	0.000398	0.679145	−0.225667
0.722793	−0.000025	0.000936	0.288066	−0.198144
0.174095	0.000007	−0.000106	0.009480	0.323571
0.077469	−0.000005	0.000079	−0.003576	0.590928
0.033610	0.000001	−0.000025	0.000920	0.245828

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−32.941430	−3.277362		−0.706586
45490.82	0.000011	−0.000004	174.0949	0.002280
10766.87	0.000094	−0.000035	51.97171	0.017969
3498.309	0.000553	−0.000204	19.44272	0.074016
1340.303	0.002518	−0.000932	8.048069	0.195991
570.6821	0.009484	−0.003529	3.470863	0.325776
261.6042	0.030150	−0.011369	1.470447	0.364192
126.6792	0.080614	−0.031122	0.592463	0.277080
63.94767	0.174215	−0.069786	0.215419	0.105863
33.20310	0.288119	−0.120614		
17.60579	0.330101	−0.145651		
9.443748	0.211805	−0.049163		
5.010148	0.057476	0.199004		
2.600078	0.005023	0.407261		
1.317443	0.000936	0.379609		
0.642767	0.000155	0.158415		
0.261221	0.000038	0.015495		

Table CLXXVII. Ni ^3F $(24s16p12d)$ basis set. Energy(E_H) = −1506.870885

	s space			
Exponent	1s	2s	3s	4s
	−305.619000	−37.917820	−4.887828	−0.276245
40843100.	0.000001	0.000000	0.000000	0.000000
6120902.	0.000005	−0.000002	0.000001	0.000000
1393820.	0.000026	−0.000008	0.000003	−0.000001
395026.2	0.000108	−0.000033	0.000012	−0.000003
128945.5	0.000396	−0.000121	0.000045	−0.000009
46575.66	0.001293	−0.000397	0.000149	−0.000031
18175.39	0.003874	−0.001192	0.000446	−0.000092
7543.199	0.010748	−0.003331	0.001250	−0.000259
3293.016	0.027675	−0.008699	0.003267	−0.000676
1499.845	0.065367	−0.021207	0.008003	−0.001662
708.0691	0.137465	−0.047412	0.018005	−0.003727
344.5831	0.242148	−0.094330	0.036418	−0.007592
172.0636	0.317967	−0.154806	0.061417	−0.012762
87.59756	0.251598	−0.172772	0.072306	−0.015304
44.93533	0.084203	−0.020536	0.008827	−0.001626
22.84855	0.006136	0.349192	−0.188565	0.040439
11.94022	0.000870	0.533981	−0.420344	0.097164
6.241623	−0.000245	0.248892	−0.227136	0.050296
3.024284	0.000074	0.027133	0.397562	−0.105465
1.478516	−0.000080	0.001189	0.651234	−0.224944
0.696625	0.000018	0.000590	0.257262	−0.185031
0.175648	−0.000007	−0.000025	0.008122	0.323530
0.077485	0.000005	0.000022	−0.002842	0.594393
0.033555	−0.000001	−0.000007	0.000726	0.244673

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−32.941730	−3.277670		−0.706924
45296.19	0.000011	−0.000004	775.4186	0.000093
10717.84	0.000095	−0.000035	234.0743	0.000892
3481.516	0.000557	−0.000206	91.05937	0.005150
1333.562	0.002540	−0.000940	40.33643	0.020305
567.6840	0.009569	−0.003560	19.12758	0.059086
260.1692	0.030413	−0.011471	9.490583	0.133919
125.9544	0.081268	−0.031381	4.836077	0.224804
63.56361	0.175389	−0.070285	2.464245	0.283258
32.99007	0.289409	−0.121214	1.235883	0.281530
17.48418	0.330061	−0.145657	0.604130	0.217240
9.371176	0.209963	−0.046842	0.283355	0.113261
4.964180	0.056106	0.203087	0.123020	0.026020
2.574640	0.004796	0.408720		
1.304974	0.000930	0.376800		
0.637095	0.000148	0.155405		
0.258232	0.000038	0.014958		

Table CLXXVIII. Ni ^3D $(20s12p9d)$ basis set. Energy(E_H) = −1506.823185

		s space		
Exponent	1s	2s	3s	4s
	−305.396200	−37.671660	−4.655030	−0.236165
4972909.	0.000009	−0.000003	0.000001	0.000000
744681.6	0.000068	−0.000021	0.000008	−0.000001
169470.8	0.000358	−0.000110	0.000041	−0.000007
48001.13	0.001508	−0.000463	0.000172	−0.000031
15658.98	0.005461	−0.001682	0.000626	−0.000113
5652.325	0.017513	−0.005446	0.002034	−0.000367
2203.844	0.049988	−0.015922	0.005949	−0.001078
913.2492	0.124070	−0.041703	0.015730	−0.002842
397.3264	0.250993	−0.094742	0.036113	−0.006564
179.6737	0.359443	−0.172132	0.068023	−0.012340
83.23984	0.275582	−0.192369	0.079631	−0.014695
37.55645	0.064991	0.054237	−0.023635	0.004620
18.12363	−0.001684	0.528164	−0.322410	0.061423
8.701685	0.001973	0.494204	−0.451124	0.092426
3.798940	−0.000907	0.084927	0.171870	−0.045681
1.784720	0.000401	−0.002837	0.721292	−0.182514
0.774064	−0.000156	0.002286	0.373990	−0.200133
0.175971	0.000059	−0.000515	0.016905	0.100530
0.085056	−0.000042	0.000397	−0.006499	0.600659
0.033374	0.000011	−0.000087	0.001551	0.422387

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−32.700010	−3.060736		−0.458019
8969.360	0.000180	−0.000066	227.1006	0.001243
2124.719	0.001580	−0.000578	67.93857	0.010395
689.5834	0.008807	−0.003252	25.79018	0.045872
262.8382	0.036238	−0.013535	10.83430	0.133624
110.7557	0.113228	−0.043753	4.813355	0.256126
49.87727	0.256578	−0.103268	2.137674	0.330608
23.37698	0.384861	−0.166103	0.914910	0.315350
11.23509	0.303392	−0.107672	0.367883	0.222265
5.291520	0.081727	0.201908	0.133679	0.085024
2.455595	0.003432	0.482581		
1.090173	0.001346	0.392527		
0.442581	0.000009	0.094716		

Table CLXXIX. Ni ^3D ($21s13p10d$) basis set. Energy(E_H) = −1506.823725

	s space			
Exponent	1s	2s	3s	4s
	−305.396400	−37.671850	−4.655221	−0.236248
8637024.	0.000004	−0.000001	0.000001	0.000000
1293279.	0.000034	−0.000010	0.000004	−0.000001
294318.1	0.000179	−0.000055	0.000020	−0.000004
83366.40	0.000758	−0.000232	0.000086	−0.000016
27198.17	0.002753	−0.000847	0.000316	−0.000057
9819.065	0.008915	−0.002753	0.001025	−0.000185
3829.676	0.026040	−0.008165	0.003053	−0.000552
1588.278	0.068193	−0.022023	0.008239	−0.001490
692.4051	0.154561	−0.053552	0.020285	−0.003674
314.4215	0.280916	−0.111569	0.042772	−0.007761
147.5250	0.348665	−0.183076	0.073314	−0.013366
70.39711	0.220969	−0.160803	0.067364	−0.012365
31.49393	0.039082	0.152552	−0.071793	0.013355
15.69449	−0.002535	0.561315	−0.372078	0.072374
7.743409	0.001628	0.408599	−0.385475	0.078159
3.413966	−0.000728	0.056880	0.286110	−0.069278
1.606831	0.000300	−0.001504	0.704151	−0.190730
0.708350	−0.000111	0.001513	0.305883	−0.177003
0.139519	0.000037	−0.000261	0.010418	0.274398
0.065525	−0.000030	0.000240	−0.004872	0.570805
0.028841	0.000010	−0.000061	0.001434	0.284001

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−32.700210	−3.060925		−0.458198
13817.53	0.000085	−0.000031	329.6683	0.000564
3271.827	0.000750	−0.000275	98.81783	0.005016
1062.507	0.004271	−0.001567	38.03799	0.024410
406.0284	0.018285	−0.006795	16.29055	0.078630
171.7943	0.061630	−0.023302	7.437544	0.179457
78.01100	0.160367	−0.063121	3.479406	0.279189
37.11006	0.302859	−0.124434	1.603745	0.315590
18.20669	0.370242	−0.162696	0.711710	0.277032
9.080722	0.224958	−0.038973	0.298440	0.180595
4.388839	0.045222	0.282931	0.114352	0.060995
2.075637	0.001824	0.478486		
0.944637	0.000838	0.327901		
0.389872	0.000062	0.065657		

Table CLXXX. Ni ^3D $(22s14p10d)$ basis set. Energy(E_H) = −1506.823843

	s space			
Exponent	1s	2s	3s	4s
	−305.396400	−37.671870	−4.655237	−0.236256
15000130.	0.000002	−0.000001	0.000000	0.000000
2245956.	0.000017	−0.000005	0.000002	0.000000
511125.4	0.000090	−0.000028	0.000010	−0.000002
144783.7	0.000380	−0.000117	0.000044	−0.000008
47239.32	0.001385	−0.000425	0.000158	−0.000029
17056.41	0.004508	−0.001389	0.000518	−0.000094
6653.656	0.013351	−0.004139	0.001542	−0.000279
2760.453	0.036054	−0.011406	0.004270	−0.000773
1204.498	0.087476	−0.028723	0.010767	−0.001947
548.0672	0.182433	−0.065232	0.024804	−0.004497
258.3212	0.299730	−0.125634	0.048496	−0.008800
125.3414	0.325533	−0.185691	0.075228	−0.013749
61.73905	0.174256	−0.125261	0.053029	−0.009716
28.36970	0.025184	0.221424	−0.108492	0.020204
14.29894	−0.001358	0.566809	−0.397017	0.077960
7.185618	0.000920	0.351417	−0.333909	0.067339
3.241734	−0.000419	0.043906	0.340117	−0.081102
1.531378	0.000147	−0.000394	0.686522	−0.191385
0.684128	−0.000059	0.001107	0.278080	−0.167381
0.138348	0.000018	−0.000146	0.008729	0.291409
0.063438	−0.000014	0.000146	−0.003822	0.576700
0.028069	0.000005	−0.000033	0.001172	0.262878

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−32.700230	−3.060942		−0.458211
20595.01	0.000042	−0.000015	329.8217	0.000563
4875.090	0.000375	−0.000137	98.86388	0.005011
1583.432	0.002167	−0.000795	38.05651	0.024389
605.8930	0.009542	−0.003522	16.29940	0.078568
257.0617	0.033761	−0.012641	7.441660	0.179381
117.1821	0.096383	−0.037062	3.480957	0.279214
56.23973	0.212071	−0.084966	1.604098	0.315697
27.90120	0.336052	−0.141817	0.711702	0.277091
14.18895	0.328572	−0.140419	0.298413	0.180569
7.269653	0.148841	0.046239	0.114349	0.060998
3.624407	0.021572	0.346418		
1.753939	0.001506	0.454763		
0.817373	0.000414	0.264542		
0.340128	0.000101	0.043371		

Table CLXXXI. Ni ^3D $(23s15p11d)$ basis set. Energy(E_H) = −1506.823959

	s space			
Exponent	1s	2s	3s	4s
	−305.396500	−37.671920	−4.655294	−0.236280
24644420.	0.000001	0.000000	0.000000	0.000000
3688394.	0.000009	−0.000003	0.000001	0.000000
838962.2	0.000048	−0.000015	0.000005	−0.000001
237570.8	0.000205	−0.000063	0.000023	−0.000004
77509.78	0.000747	−0.000229	0.000085	−0.000015
27990.05	0.002438	−0.000749	0.000279	−0.000050
10921.45	0.007268	−0.002245	0.000838	−0.000151
4532.318	0.019963	−0.006228	0.002322	−0.000420
1978.344	0.050222	−0.016080	0.006027	−0.001091
900.7662	0.113075	−0.038018	0.014298	−0.002586
424.9766	0.215931	−0.080558	0.030779	−0.005587
206.7016	0.315446	−0.142570	0.055606	−0.010094
103.1101	0.289449	−0.183101	0.075274	−0.013804
52.20754	0.121711	−0.072766	0.031182	−0.005674
25.20462	0.012997	0.297622	−0.152840	0.028589
12.88244	0.000072	0.558131	−0.416839	0.082684
6.592824	0.000166	0.289609	−0.269482	0.053714
3.062654	−0.000099	0.032122	0.391941	−0.092694
1.457607	−0.000002	0.000567	0.663946	−0.190863
0.660787	−0.000009	0.000750	0.251422	−0.157857
0.138684	0.000002	−0.000056	0.007425	0.297211
0.062642	−0.000001	0.000075	−0.003000	0.582021
0.027706	0.000000	−0.000011	0.000947	0.253452

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−32.700290	−3.060997		−0.458263
30391.10	0.000021	−0.000008	472.7312	0.000260
7192.246	0.000191	−0.000070	142.0648	0.002404
2336.258	0.001111	−0.000407	55.05260	0.012745
894.6209	0.004991	−0.001836	23.99379	0.044651
380.3611	0.018286	−0.006795	11.14180	0.115602
173.9080	0.055553	−0.021020	5.387016	0.214729
83.91479	0.136751	−0.053535	2.615866	0.286058
42.03956	0.258190	−0.105316	1.243849	0.293782
21.59655	0.345237	−0.149515	0.570251	0.241377
11.29194	0.269081	−0.097964	0.248413	0.146398
5.879569	0.090996	0.133989	0.099808	0.043964
2.996316	0.009411	0.388098		
1.483470	0.001269	0.415653		
0.706551	0.000220	0.205557		
0.293355	0.000094	0.027236		

Table CLXXXII. Cu ^2S $(20s12p9d)$ basis set. Energy(E_H) = −1638.962880

	s space			
Exponent	1s	2s	3s	4s
	−328.792600	−40.818590	−5.011612	−0.238329
9148883.	0.000005	−0.000001	0.000001	0.000000
1369956.	0.000035	−0.000011	0.000004	−0.000001
311782.6	0.000182	−0.000056	0.000021	−0.000004
88318.80	0.000770	−0.000237	0.000089	−0.000015
28815.53	0.002798	−0.000864	0.000324	−0.000056
10403.46	0.009056	−0.002808	0.001050	−0.000182
4057.791	0.026441	−0.008330	0.003129	−0.000544
1682.974	0.069180	−0.022454	0.008439	−0.001458
733.7543	0.156480	−0.054566	0.020769	−0.003619
333.2677	0.283188	−0.113392	0.043699	−0.007559
156.4338	0.348347	−0.185125	0.074595	−0.013136
74.69721	0.217298	−0.158739	0.066974	−0.011555
33.32262	0.037238	0.166012	−0.079477	0.013602
16.62237	−0.002579	0.568082	−0.384797	0.073169
8.208260	0.001558	0.395061	−0.372597	0.069755
3.609400	−0.000677	0.051919	0.319617	−0.068722
1.683449	0.000259	−0.001039	0.704002	−0.193438
0.733757	−0.000084	0.001224	0.280302	−0.151634
0.110207	0.000014	−0.000094	0.005123	0.558396
0.038786	−0.000006	0.000041	−0.001364	0.558881

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−35.617550	−3.324458		−0.490887
9713.253	0.000178	−0.000066	249.3497	0.001244
2300.889	0.001569	−0.000578	74.63837	0.010457
746.7706	0.008754	−0.003257	28.37641	0.046441
284.6806	0.036082	−0.013578	11.94893	0.135361
119.9999	0.112988	−0.044000	5.317646	0.258371
54.07386	0.256651	−0.104177	2.364417	0.331379
25.37321	0.385161	−0.167690	1.012386	0.313637
12.20962	0.302937	−0.107122	0.406773	0.219475
5.757421	0.081544	0.204961	0.147331	0.083664
2.673402	0.003544	0.483002		
1.186835	0.001370	0.390189		
0.481593	0.000022	0.094083		

Table CLXXXIII. Cu ^2S ($22s14p10d$) basis set. Energy(E_H) = -1638.963529

	s space			
Exponent	1s	2s	3s	4s
	−328.792900	−40.818860	−5.011877	−0.238452
16057550.	0.000002	−0.000001	0.000000	0.000000
2404206.	0.000017	−0.000005	0.000002	0.000000
547134.0	0.000090	−0.000028	0.000010	−0.000002
154981.8	0.000382	−0.000117	0.000044	−0.000008
50565.79	0.001390	−0.000428	0.000160	−0.000028
18257.16	0.004523	−0.001399	0.000524	−0.000091
7121.958	0.013394	−0.004170	0.001560	−0.000271
2954.700	0.036170	−0.011494	0.004322	−0.000750
1289.246	0.087746	−0.028948	0.010902	−0.001891
586.6445	0.182933	−0.065756	0.025122	−0.004368
276.5331	0.300237	−0.126618	0.049126	−0.008552
134.2132	0.325271	−0.186864	0.076127	−0.013342
66.15410	0.173304	−0.124736	0.053166	−0.009354
30.43267	0.024818	0.226744	−0.112496	0.020139
15.35577	−0.001354	0.568792	−0.403606	0.075983
7.722872	0.000893	0.346371	−0.327243	0.063143
3.485634	−0.000404	0.042554	0.353353	−0.080569
1.642127	0.000140	−0.000270	0.684111	−0.182422
0.731466	−0.000055	0.001052	0.269523	−0.159096
0.141724	0.000016	−0.000138	0.007922	0.294113
0.064323	−0.000013	0.000113	−0.003650	0.572702
0.028406	0.000004	−0.000039	0.001104	0.259691

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−35.617840	−3.324723		−0.491138
22287.62	0.000042	−0.000015	361.8313	0.000564
5275.873	0.000373	−0.000137	108.5176	0.005037
1713.639	0.002154	−0.000796	41.80954	0.024663
655.7449	0.009496	−0.003531	17.94168	0.079739
278.2540	0.033649	−0.012694	8.206966	0.181580
126.8780	0.096248	−0.037299	3.843896	0.281134
60.92106	0.212236	−0.085741	1.772723	0.315624
30.24838	0.336606	−0.143363	0.786511	0.274869
15.39702	0.328308	−0.140811	0.329431	0.177893
7.894000	0.148129	0.049091	0.125769	0.059914
3.939187	0.021470	0.348978		
1.907293	0.001572	0.453326		
0.888751	0.000432	0.262213		
0.369894	0.000108	0.043000		

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Table CLXXXIV. Cu ^2S $(23s15p11d)$ basis set. Energy(E_H) = −1638.963664

	s space			
Exponent	1s	2s	3s	4s
	−328.792900	−40.818920	−5.011943	−0.238479
26284110.	0.000001	0.000000	0.000000	0.000000
3934593.	0.000009	−0.000003	0.000001	0.000000
895242.5	0.000049	−0.000015	0.000006	−0.000001
253557.7	0.000206	−0.000064	0.000024	−0.000004
82725.46	0.000752	−0.000232	0.000087	−0.000015
29869.43	0.002456	−0.000757	0.000283	−0.000049
11652.75	0.007322	−0.002271	0.000851	−0.000148
4835.009	0.020112	−0.006302	0.002361	−0.000409
2110.132	0.050594	−0.016275	0.006127	−0.001064
960.6121	0.113869	−0.038484	0.014542	−0.002523
453.1518	0.217181	−0.081531	0.031302	−0.005449
220.3899	0.316311	−0.144108	0.056519	−0.009844
109.9379	0.288377	−0.184126	0.076152	−0.013391
55.68357	0.119665	−0.070055	0.030249	−0.005289
26.95586	0.012453	0.305441	−0.159139	0.028616
13.79255	0.000113	0.558460	−0.422990	0.080435
7.063698	0.000129	0.282869	−0.259152	0.049333
3.286432	−0.000084	0.030712	0.405548	−0.091734
1.560907	−0.000007	0.000678	0.659821	−0.181684
0.705849	−0.000006	0.000703	0.242757	−0.149851
0.142258	0.000001	−0.000053	0.006705	0.298656
0.063604	−0.000001	0.000045	−0.002862	0.578665
0.028048	0.000000	−0.000016	0.000883	0.250829

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−35.617910	−3.324786		−0.491198
32794.52	0.000021	−0.000008	0.109507	0.043038
7760.899	0.000191	−0.000070	0.273592	0.143757
2520.930	0.001110	−0.000410	0.628796	0.238722
965.3069	0.004989	−0.001849	1.371903	0.292881
410.4222	0.018302	−0.006852	2.883906	0.287444
187.6788	0.055675	−0.021229	5.933472	0.217203
90.58511	0.137215	−0.054155	12.25498	0.117501
45.40552	0.259216	−0.106690	26.34210	0.045395
23.34720	0.345743	−0.151065	60.36477	0.012890
12.21776	0.267686	−0.096535	155.6931	0.002419
6.364777	0.089762	0.138739	517.8221	0.000261
3.245528	0.009276	0.390449		
1.607599	0.001309	0.412822		
0.765723	0.000233	0.202468		
0.317997	0.000098	0.026716		

Table CLXXXV. Cu ^2S $(23s15p8d)$ basis set. Energy(E_H) = −1638.962294

	s space			
Exponent	1s	2s	3s	4s
	−328.792300	−40.818200	−5.011181	−0.238183
26448990.	0.000001	0.000000	0.000000	0.000000
3954373.	0.000009	−0.000003	0.000001	0.000000
898801.5	0.000049	−0.000015	0.000006	−0.000001
254395.7	0.000206	−0.000063	0.000024	−0.000004
82974.41	0.000750	−0.000231	0.000086	−0.000015
29956.40	0.002447	−0.000755	0.000282	−0.000049
11686.86	0.007295	−0.002263	0.000848	−0.000147
4849.428	0.020038	−0.006279	0.002352	−0.000407
2116.564	0.050413	−0.016215	0.006104	−0.001059
963.6234	0.113492	−0.038346	0.014489	−0.002512
454.6030	0.216624	−0.081271	0.031200	−0.005427
221.0992	0.315998	−0.143796	0.056385	−0.009814
110.2877	0.288933	−0.184156	0.076147	−0.013379
55.85414	0.120482	−0.071138	0.030706	−0.005368
27.03009	0.012627	0.303659	−0.158013	0.028393
13.82893	0.000104	0.558697	−0.422513	0.080259
7.081041	0.000135	0.284436	−0.260907	0.049668
3.291549	−0.000086	0.031020	0.404124	−0.091384
1.563246	−0.000006	0.000646	0.660393	−0.181469
0.706702	−0.000007	0.000715	0.243607	−0.150061
0.142425	0.000001	−0.000056	0.006763	0.296065
0.063804	−0.000001	0.000047	−0.002889	0.578938
0.028090	0.000000	−0.000017	0.000884	0.252976

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−35.617210	−3.324055		−0.490458
33073.52	0.000021	−0.000008	0.176981	0.117256
7827.020	0.000188	−0.000069	0.518084	0.269362
2542.446	0.001094	−0.000404	1.348977	0.352554
973.6580	0.004917	−0.001822	3.279369	0.333380
414.0197	0.018048	−0.006755	7.731246	0.215303
189.3389	0.054967	−0.020953	18.78703	0.085985
91.38806	0.135800	−0.053568	50.48152	0.021460
45.80218	0.257590	−0.105957	169.2545	0.002791
23.53999	0.345689	−0.150928		
12.30921	0.269967	−0.098375		
6.406570	0.091391	0.136189		
3.261947	0.009501	0.390222		
1.613465	0.001319	0.414193		
0.767912	0.000234	0.203578		
0.319115	0.000099	0.026998		

Table CLXXXVI. Cu ^2D $(20s12p9d)$ basis set. Energy$(E_H) = -1638.949295$

	s space			
Exponent	1s	2s	3s	4s
	−329.034200	−41.084540	−5.260407	−0.284664
5430321.	0.000009	−0.000003	0.000001	0.000000
813166.5	0.000067	−0.000020	0.000008	−0.000002
185054.4	0.000350	−0.000108	0.000041	−0.000008
52414.66	0.001476	−0.000455	0.000171	−0.000035
17098.68	0.005345	−0.001653	0.000622	−0.000127
6171.994	0.017149	−0.005354	0.002020	−0.000412
2406.481	0.048998	−0.015668	0.005916	−0.001206
997.2584	0.121900	−0.041090	0.015655	−0.003196
433.9289	0.247764	−0.093690	0.036092	−0.007375
196.2869	0.358203	−0.171159	0.068293	−0.014028
91.04280	0.279608	−0.194887	0.081589	−0.016837
41.38425	0.068576	0.044044	−0.019348	0.003948
19.93278	−0.001228	0.521759	−0.320280	0.069795
9.581891	0.001911	0.502501	−0.461183	0.105100
4.234516	−0.000877	0.090591	0.153947	−0.043141
1.985814	0.000375	−0.002186	0.730162	−0.218375
0.867083	−0.000142	0.002147	0.382698	−0.228861
0.181339	0.000049	−0.000430	0.014928	0.312697
0.083657	−0.000038	0.000335	−0.006993	0.570242
0.036267	0.000012	−0.000105	0.001835	0.267774

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−35.878860	−3.556713		−0.740016
9902.688	0.000172	−0.000064	281.0982	0.001011
2345.723	0.001517	−0.000563	84.19383	0.008692
761.3584	0.008476	−0.003176	32.17398	0.039850
290.2819	0.035007	−0.013268	13.63207	0.120578
122.3838	0.110072	−0.043136	6.131970	0.244498
55.17048	0.251867	−0.102900	2.780154	0.332131
25.90215	0.382882	−0.167580	1.226604	0.325377
12.47785	0.308432	−0.113510	0.514703	0.221074
5.910417	0.086769	0.193208	0.195953	0.073830
2.755762	0.004148	0.482586		
1.234408	0.001369	0.399186		
0.508187	−0.000022	0.094323		

Table CLXXXVII. Cu ^2D ($21s13p10d$) basis set. Energy(E_H) = -1638.949796

	s space			
Exponent	1s	2s	3s	4s
	−329.034300	−41.084670	−5.260524	−0.284709
9534997.	0.000004	−0.000001	0.000001	0.000000
1427682.	0.000033	−0.000010	0.000004	−0.000001
324895.8	0.000173	−0.000053	0.000020	−0.000004
92026.07	0.000731	−0.000225	0.000085	−0.000017
30023.02	0.002659	−0.000821	0.000309	−0.000063
10838.78	0.008611	−0.002670	0.001004	−0.000205
4227.325	0.025178	−0.007923	0.002993	−0.000611
1753.152	0.066083	−0.021409	0.008094	−0.001649
764.2596	0.150501	−0.052204	0.019967	−0.004082
347.0302	0.276130	−0.109516	0.042425	−0.008667
162.8066	0.349134	−0.181802	0.073433	−0.015129
77.71823	0.228579	−0.166715	0.070663	−0.014556
35.08426	0.043006	0.132768	−0.063025	0.013027
17.52766	−0.002477	0.552449	−0.364305	0.080447
8.666210	0.001719	0.427021	−0.405250	0.092038
3.889212	−0.000782	0.065503	0.243788	−0.065155
1.846273	0.000328	−0.001323	0.711257	−0.221193
0.826276	−0.000125	0.001642	0.336514	−0.212358
0.182717	0.000041	−0.000286	0.011919	0.321257
0.082039	−0.000030	0.000215	−0.005086	0.579959
0.035508	0.000010	−0.000068	0.001343	0.253005

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−35.878990	−3.556829		−0.740130
15247.67	0.000081	−0.000030	410.6458	0.000450
3610.418	0.000720	−0.000268	123.2549	0.004084
1172.491	0.004109	−0.001530	47.62274	0.020637
448.1311	0.017643	−0.006652	20.56372	0.068812
189.6788	0.059737	−0.022915	9.470416	0.164832
86.18436	0.156604	−0.062527	4.497504	0.271784
41.04592	0.298874	−0.124657	2.119450	0.321569
20.16871	0.370740	−0.165304	0.970282	0.286586
10.07839	0.230769	−0.045180	0.423580	0.177023
4.890862	0.048467	0.276875	0.168926	0.051921
2.325085	0.002053	0.481071		
1.068268	0.000880	0.332294		
0.446196	0.000024	0.064197		

Table CLXXXVIII. Cu ^2D ($21s14p10d$) basis set. Energy(E_H) = -1638.949864

	s space			
Exponent	1s	2s	3s	4s
	−329.034300	−41.084680	−5.260532	−0.284715
9532057.	0.000004	−0.000001	0.000001	0.000000
1427256.	0.000033	−0.000010	0.000004	−0.000001
324800.7	0.000173	−0.000053	0.000020	−0.000004
91999.50	0.000732	−0.000225	0.000085	−0.000017
30014.50	0.002660	−0.000821	0.000309	−0.000063
10835.77	0.008614	−0.002671	0.001005	−0.000205
4226.179	0.025187	−0.007925	0.002994	−0.000611
1752.681	0.066103	−0.021416	0.008097	−0.001650
764.0548	0.150539	−0.052220	0.019973	−0.004083
346.9386	0.276175	−0.109541	0.042435	−0.008669
162.7649	0.349129	−0.181823	0.073443	−0.015132
77.69855	0.228508	−0.166667	0.070643	−0.014551
35.07209	0.042968	0.132974	−0.063127	0.013048
17.52200	−0.002480	0.552532	−0.364434	0.080481
8.663675	0.001719	0.426825	−0.405078	0.091997
3.888016	−0.000782	0.065433	0.244082	−0.065227
1.845796	0.000328	−0.001323	0.711182	−0.221209
0.826125	−0.000125	0.001641	0.336354	−0.212297
0.182745	0.000041	−0.000286	0.011898	0.321177
0.082047	−0.000030	0.000215	−0.005066	0.580031
0.035509	0.000010	−0.000068	0.001337	0.253026

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−35.879010	−3.556840		−0.740137
22760.57	0.000040	−0.000015	410.5321	0.000450
5387.679	0.000360	−0.000133	123.2214	0.004086
1749.945	0.002078	−0.000774	47.60979	0.020647
669.6653	0.009172	−0.003434	20.55766	0.068845
284.1948	0.032568	−0.012372	9.466730	0.164926
129.6077	0.093526	−0.036477	4.494962	0.271917
62.25415	0.207647	−0.084413	2.117919	0.321608
30.92964	0.332968	−0.142580	0.969574	0.286466
15.75827	0.331483	−0.144306	0.423352	0.176876
8.094211	0.155039	0.039022	0.168863	0.051883
4.046921	0.023747	0.342258		
1.967869	0.001566	0.459554		
0.925295	0.000450	0.267532		
0.388098	0.000065	0.041682		

Table CLXXXIX. Cu ^2D $(22s14p10d)$ basis set. Energy(E_H) = −1638.949916

	s space			
Exponent	1s	2s	3s	4s
	−329.034400	−41.084680	−5.260537	−0.284715
16665490.	0.000002	−0.000001	0.000000	0.000000
2495213.	0.000016	−0.000005	0.000002	0.000000
567850.7	0.000086	−0.000026	0.000010	−0.000002
160853.1	0.000364	−0.000112	0.000042	−0.000009
52481.86	0.001327	−0.000409	0.000154	−0.000031
18948.85	0.004319	−0.001336	0.000503	−0.000103
7391.655	0.012800	−0.003984	0.001499	−0.000305
3066.517	0.034623	−0.010988	0.004155	−0.000848
1337.994	0.084288	−0.027740	0.010508	−0.002140
608.7830	0.177015	−0.063269	0.024289	−0.004970
286.8980	0.294791	−0.122996	0.047958	−0.009797
139.1530	0.328547	−0.185098	0.075594	−0.015616
68.49455	0.183685	−0.134106	0.057474	−0.011805
31.60108	0.028487	0.200111	−0.098799	0.020560
15.99158	−0.001545	0.561272	−0.390359	0.086969
8.056510	0.001069	0.371196	−0.356991	0.080673
3.690329	−0.000490	0.051268	0.298897	−0.078853
1.762902	0.000183	−0.000365	0.695284	−0.222113
0.801269	−0.000074	0.001248	0.308591	−0.201844
0.184243	0.000023	−0.000182	0.010400	0.321824
0.081793	−0.000016	0.000135	−0.004159	0.585095
0.035303	0.000005	−0.000043	0.001090	0.249388

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−35.879010	−3.556843		−0.740141
22761.04	0.000040	−0.000015	410.5438	0.000450
5387.778	0.000360	−0.000133	123.2233	0.004086
1749.985	0.002078	−0.000774	47.61017	0.020646
669.6867	0.009171	−0.003434	20.55782	0.068844
284.2077	0.032565	−0.012371	9.466728	0.164930
129.6164	0.093514	−0.036472	4.494862	0.271928
62.25991	0.207623	−0.084403	2.117841	0.321608
30.93249	0.332965	−0.142576	0.969547	0.286458
15.75914	0.331516	−0.144324	0.423344	0.176871
8.094204	0.155054	0.039033	0.168861	0.051880
4.046555	0.023743	0.342319		
1.967644	0.001565	0.459533		
0.925232	0.000450	0.267483		
0.388095	0.000065	0.041679		

Table CXC. Cu ^2D $(23s15p11d)$ basis set. Energy(E_H) = −1638.950018

	s space			
Exponent	1s	2s	3s	4s
	−329.034400	−41.084720	−5.260571	−0.284729
27903820.	0.000001	0.000000	0.000000	0.000000
4177473.	0.000009	−0.000003	0.000001	0.000000
950685.3	0.000045	−0.000014	0.000005	−0.000001
269302.1	0.000191	−0.000059	0.000022	−0.000005
87868.25	0.000698	−0.000215	0.000081	−0.000016
31726.78	0.002278	−0.000702	0.000264	−0.000054
12377.02	0.006798	−0.002108	0.000794	−0.000162
5135.356	0.018702	−0.005853	0.002205	−0.000449
2241.272	0.047201	−0.015145	0.005733	−0.001171
1020.471	0.106957	−0.035949	0.013656	−0.002782
481.5371	0.206810	−0.076768	0.029602	−0.006065
234.2997	0.309562	−0.137922	0.054262	−0.011088
116.9615	0.297557	−0.183744	0.076025	−0.015759
59.25351	0.136145	−0.090104	0.039124	−0.007965
28.46521	0.016636	0.267996	−0.137724	0.028837
14.58789	−0.000288	0.558066	−0.410227	0.092211
7.476286	0.000372	0.316329	−0.302792	0.067760
3.507086	−0.000186	0.039440	0.347507	−0.091066
1.688567	0.000038	0.000464	0.677154	−0.222230
0.778728	−0.000023	0.000911	0.283806	−0.192027
0.185678	0.000006	−0.000097	0.009199	0.321448
0.081764	−0.000004	0.000073	−0.003464	0.588853
0.035206	0.000001	−0.000023	0.000901	0.247817

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−35.879050	−3.556876		−0.740173
33468.80	0.000021	−0.000008	591.3193	0.000205
7920.508	0.000184	−0.000068	177.9997	0.001920
2572.781	0.001071	−0.000399	69.11027	0.010504
985.1906	0.004820	−0.001799	30.31889	0.038187
418.9109	0.017711	−0.006677	14.18423	0.102622
191.5823	0.054024	−0.020740	6.929321	0.201629
92.48285	0.133822	−0.053149	3.421509	0.283659
46.37237	0.254828	−0.105524	1.665020	0.302649
23.85367	0.344407	−0.151370	0.787632	0.249041
12.49363	0.272831	−0.102167	0.356243	0.140967
6.523913	0.095039	0.128953	0.148118	0.036645
3.333676	0.010375	0.387678		
1.658572	0.001286	0.420665		
0.796541	0.000229	0.205125		
0.331019	0.000063	0.025133		

Table CXCI. Cu ^2D $(24s16p12d)$ basis set. Energy(E_H) = −1638.950055

	s space			
Exponent	1s	2s	3s	4s
	−329.034400	−41.084730	−5.260584	−0.284734
43655530.	0.000001	0.000000	0.000000	0.000000
6539971.	0.000005	−0.000002	0.000001	0.000000
1488716.	0.000026	−0.000008	0.000003	−0.000001
421799.5	0.000109	−0.000034	0.000013	−0.000003
137663.0	0.000398	−0.000123	0.000046	−0.000009
49725.96	0.001302	−0.000401	0.000151	−0.000031
19408.23	0.003897	−0.001204	0.000453	−0.000092
8056.884	0.010808	−0.003364	0.001268	−0.000259
3518.184	0.027816	−0.008782	0.003313	−0.000674
1602.793	0.065669	−0.021405	0.008114	−0.001658
756.8437	0.138013	−0.047850	0.018258	−0.003719
368.4019	0.242853	−0.095176	0.036923	−0.007576
183.9938	0.318222	−0.156067	0.062262	−0.012731
93.68162	0.250783	−0.173439	0.073016	−0.015212
48.04983	0.083111	−0.017984	0.007756	−0.001371
24.50472	0.005852	0.354768	−0.194243	0.041039
12.82532	0.000892	0.533056	−0.424333	0.096577
6.710963	−0.000266	0.244427	−0.218802	0.047442
3.259019	0.000083	0.026353	0.406327	−0.106090
1.592732	−0.000082	0.001248	0.647428	−0.221135
0.749517	0.000019	0.000564	0.252351	−0.178690
0.187394	−0.000007	−0.000018	0.007852	0.320627
0.081854	0.000005	0.000018	−0.002736	0.592510
0.035156	−0.000001	−0.000006	0.000703	0.247155

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−35.879060	−3.556888		−0.740185
48218.41	0.000011	−0.000004	0.131332	0.025759
11420.55	0.000097	−0.000036	0.304193	0.111465
3713.569	0.000568	−0.000211	0.651502	0.213974
1423.762	0.002582	−0.000963	1.337379	0.279219
606.6041	0.009715	−0.003642	2.671733	0.283980
278.2564	0.030843	−0.011723	5.246289	0.228045
134.8449	0.082294	−0.032039	10.28998	0.137411
68.12254	0.177224	−0.071645	20.70706	0.061043
35.40088	0.291330	−0.123238	43.61334	0.020974
18.79029	0.329315	−0.146316	98.38874	0.005313
10.08356	0.206588	−0.042399	252.7590	0.000920
5.346120	0.054327	0.209844	836.9257	0.000096
2.775228	0.004667	0.410257		
1.407564	0.000949	0.371910		
0.687213	0.000162	0.151472		
0.278217	0.000040	0.014451		

Table CXCII. Zn ^1S $(20s12p9d)$ basis set. Energy(E_H) = −1777.847233

	s space			
Exponent	1s	2s	3s	4s
	−353.304300	−44.361500	−5.637602	−0.292423
5820021.	0.000008	−0.000003	0.000001	0.000000
871523.4	0.000067	−0.000020	0.000008	−0.000002
198335.0	0.000349	−0.000108	0.000041	−0.000008
56176.31	0.001474	−0.000456	0.000172	−0.000035
18325.82	0.005338	−0.001658	0.000626	−0.000125
6614.955	0.017127	−0.005369	0.002033	−0.000407
2579.199	0.048941	−0.015712	0.005955	−0.001193
1068.849	0.121793	−0.041226	0.015767	−0.003164
465.1045	0.247659	−0.094064	0.036376	−0.007305
210.4130	0.358243	−0.171996	0.068924	−0.013915
97.61629	0.279817	−0.195852	0.082381	−0.016708
44.38020	0.068575	0.045328	−0.020112	0.004035
21.42308	−0.001311	0.524444	−0.325257	0.069700
10.30891	0.001914	0.500614	−0.460287	0.103019
4.553645	−0.000876	0.089456	0.163542	−0.044708
2.132821	0.000374	−0.002146	0.729743	−0.215057
0.929697	−0.000140	0.002112	0.376948	−0.222038
0.192147	0.000048	−0.000413	0.014362	0.311719
0.087595	−0.000036	0.000320	−0.006714	0.569208
0.037702	0.000012	−0.000101	0.001780	0.267779

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−38.924600	−3.839164		−0.782332
10684.58	0.000171	−0.000064	305.0115	0.001023
2530.903	0.001509	−0.000564	91.40003	0.008816
821.4820	0.008437	−0.003181	34.95829	0.040581
313.2522	0.034897	−0.013310	14.83697	0.122700
132.1094	0.109933	−0.043365	6.680748	0.247094
59.58751	0.252066	−0.103729	3.029026	0.332771
28.00399	0.383254	−0.169009	1.334839	0.323286
13.50425	0.307877	−0.112848	0.558608	0.218840
6.401881	0.086419	0.196353	0.211743	0.073388
2.985769	0.004227	0.483030		
1.336902	0.001393	0.396755		
0.549961	−0.000008	0.093778		

Table CXCIII. Zn ^1S ($21s13p10d$) basis set. Energy(E_H) = −1777.847799

	s space			
Exponent	1s	2s	3s	4s
	−353.304400	−44.361640	−5.637736	−0.292473
10231420.	0.000004	−0.000001	0.000001	0.000000
1531819.	0.000033	−0.000010	0.000004	−0.000001
348565.5	0.000173	−0.000053	0.000020	−0.000004
98723.08	0.000730	−0.000225	0.000085	−0.000017
32205.74	0.002652	−0.000822	0.000311	−0.000062
11626.09	0.008591	−0.002675	0.001010	−0.000202
4534.156	0.025125	−0.007937	0.003009	−0.000603
1880.320	0.065962	−0.021456	0.008142	−0.001631
819.6816	0.150298	−0.052351	0.020099	−0.004038
372.2092	0.275947	−0.109922	0.042752	−0.008583
174.6407	0.349215	−0.182658	0.074095	−0.015003
83.39604	0.228913	−0.167564	0.071385	−0.014453
37.67471	0.043091	0.134417	−0.064419	0.013098
18.85039	−0.002519	0.554366	−0.369039	0.080112
9.328297	0.001714	0.425043	−0.403033	0.089889
4.188028	−0.000776	0.064769	0.252041	−0.066060
1.984683	0.000324	−0.001238	0.710110	−0.217505
0.886390	−0.000122	0.001605	0.331784	−0.206081
0.193689	0.000039	−0.000272	0.011521	0.318955
0.086107	−0.000029	0.000204	−0.004917	0.578425
0.036990	0.000009	−0.000065	0.001308	0.254642

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−38.924750	−3.839296		−0.782463
16447.98	0.000081	−0.000030	445.1670	0.000456
3894.535	0.000716	−0.000268	133.6740	0.004144
1264.745	0.004090	−0.001533	51.67507	0.021014
483.4198	0.017581	−0.006670	22.34064	0.070225
204.6556	0.059628	−0.023021	10.30273	0.167474
93.02052	0.156621	−0.062955	4.894923	0.273930
44.32946	0.299363	−0.125829	2.305779	0.321232
21.80332	0.370853	−0.166381	1.053945	0.284096
10.90462	0.229972	−0.043416	0.458837	0.175037
5.297006	0.048212	0.279770	0.182207	0.051564
2.518990	0.002137	0.480501		
1.156829	0.000897	0.330055		
0.483010	0.000035	0.063890		

Table CXCIV. Zn ^1S $(21s14p8d)$ basis set. Energy(E_H) = −1777.846810

	s space			
Exponent	1s	2s	3s	4s
	−353.304100	−44.361240	−5.637319	−0.292330
10221690.	0.000004	−0.000001	0.000001	0.000000
1530505.	0.000033	−0.000010	0.000004	−0.000001
348296.2	0.000173	−0.000053	0.000020	−0.000004
98654.21	0.000730	−0.000226	0.000085	−0.000017
32185.40	0.002654	−0.000823	0.000311	−0.000062
11619.44	0.008597	−0.002676	0.001011	−0.000202
4531.799	0.025140	−0.007942	0.003011	−0.000604
1879.427	0.065994	−0.021467	0.008146	−0.001631
819.3251	0.150354	−0.052374	0.020108	−0.004039
372.0624	0.276002	−0.109955	0.042765	−0.008584
174.5791	0.349195	−0.182679	0.074105	−0.015002
83.36956	0.228814	−0.167499	0.071358	−0.014444
37.66053	0.043046	0.134650	−0.064537	0.013120
18.84386	−0.002521	0.554437	−0.369160	0.080122
9.325702	0.001714	0.424822	−0.402839	0.089826
4.187245	−0.000776	0.064712	0.252210	−0.066090
1.984502	0.000324	−0.001235	0.709982	−0.217411
0.886391	−0.000122	0.001604	0.331775	−0.206020
0.193760	0.000039	−0.000272	0.011528	0.318038
0.086206	−0.000029	0.000204	−0.004911	0.578594
0.037006	0.000009	−0.000065	0.001301	0.255332

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−38.924370	−3.838904		−0.782027
24411.98	0.000041	−0.000015	205.6412	0.002342
5778.518	0.000361	−0.000135	61.45895	0.018600
1876.862	0.002088	−0.000782	23.06164	0.077076
718.2361	0.009221	−0.003475	9.580108	0.201974
304.8327	0.032773	−0.012530	4.134770	0.329442
139.0453	0.094179	−0.036985	1.747885	0.361005
66.80417	0.209131	−0.085647	0.699673	0.271708
33.20699	0.334570	−0.144492	0.251641	0.104990
16.92816	0.330356	−0.143951		
8.696229	0.152351	0.044604		
4.350510	0.022977	0.347041		
2.116523	0.001617	0.457118		
0.995387	0.000453	0.262849		
0.417614	0.000073	0.040693		

Table CXCV. Zn ^1S $(22s14p10d)$ basis set. Energy(E_H) = −1777.847927

	s space			
Exponent	1s	2s	3s	4s
	−353.304500	−44.361650	−5.637750	−0.292479
17852930.	0.000002	−0.000001	0.000000	0.000000
2673038.	0.000016	−0.000005	0.000002	0.000000
608324.4	0.000086	−0.000027	0.000010	−0.000002
172317.6	0.000364	−0.000113	0.000042	−0.000008
56222.69	0.001326	−0.000410	0.000155	−0.000031
20299.85	0.004315	−0.001340	0.000507	−0.000102
7918.871	0.012789	−0.003996	0.001510	−0.000302
3285.340	0.034595	−0.011024	0.004184	−0.000839
1433.524	0.084235	−0.027837	0.010584	−0.002119
652.2889	0.176950	−0.063522	0.024479	−0.004923
307.4360	0.294772	−0.123565	0.048379	−0.009713
149.1466	0.328605	−0.186033	0.076310	−0.015494
73.45108	0.183733	−0.134541	0.057979	−0.011706
33.92562	0.028456	0.202637	−0.101049	0.020686
17.18947	−0.001563	0.562794	−0.395075	0.086522
8.666595	0.001058	0.368732	−0.353421	0.078409
3.972505	−0.000483	0.050558	0.306999	−0.079508
1.894665	0.000180	−0.000285	0.693529	−0.218242
0.859385	−0.000072	0.001214	0.304046	−0.195744
0.195256	0.000022	−0.000170	0.010050	0.319523
0.085854	−0.000016	0.000126	−0.004023	0.583375
0.036781	0.000005	−0.000040	0.001063	0.251127

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−38.924770	−3.839311		−0.782474
24553.68	0.000040	−0.000015	445.0709	0.000456
5812.323	0.000358	−0.000134	133.6463	0.004145
1887.932	0.002067	−0.000774	51.66499	0.021020
722.5141	0.009131	−0.003440	22.33620	0.070247
306.6721	0.032469	−0.012412	10.29983	0.167550
139.8981	0.093399	−0.036667	4.892719	0.274046
67.22655	0.207782	−0.085065	2.304407	0.321262
33.42459	0.333491	−0.143929	1.053322	0.283993
17.04301	0.331289	−0.144656	0.458642	0.174919
8.758800	0.154370	0.041604	0.182152	0.051535
4.381915	0.023629	0.344586		
2.131359	0.001629	0.458097		
1.001793	0.000467	0.265555		
0.420304	0.000072	0.041532		

Table CXCVI. Zn ^1S $(22s15p8d)$ basis set. Energy$(E_H) = -1777.846893$

	s space			
Exponent	1s	2s	3s	4s
	−353.304200	−44.361250	−5.637329	−0.292333
17825590.	0.000002	−0.000001	0.000000	0.000000
2669077.	0.000016	−0.000005	0.000002	0.000000
607450.2	0.000086	−0.000027	0.000010	−0.000002
172079.5	0.000365	−0.000113	0.000043	−0.000008
56148.56	0.001328	−0.000411	0.000155	−0.000031
20274.42	0.004322	−0.001342	0.000508	−0.000102
7909.451	0.012807	−0.004002	0.001512	−0.000303
3281.632	0.034639	−0.011038	0.004189	−0.000840
1431.995	0.084326	−0.027869	0.010597	−0.002121
651.6360	0.177094	−0.063583	0.024503	−0.004927
307.1495	0.294887	−0.123647	0.048413	−0.009718
149.0193	0.328505	−0.186060	0.076325	−0.015493
73.39564	0.183487	−0.134335	0.057894	−0.011686
33.90186	0.028378	0.203117	−0.101315	0.020737
17.17778	−0.001558	0.562859	−0.395274	0.086548
8.661600	0.001055	0.368300	−0.353011	0.078299
3.970989	−0.000482	0.050459	0.307362	−0.079587
1.894139	0.000179	−0.000279	0.693334	−0.218139
0.859280	−0.000072	0.001212	0.303925	−0.195657
0.195384	0.000022	−0.000170	0.010055	0.318408
0.085982	−0.000016	0.000126	−0.004018	0.583535
0.036808	0.000005	−0.000040	0.001057	0.252035

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−38.924390	−3.838912		−0.782034
36051.13	0.000020	−0.000008	205.6247	0.002342
8531.933	0.000183	−0.000068	61.45387	0.018603
2771.571	0.001068	−0.000400	23.05951	0.077087
1061.409	0.004808	−0.001806	9.579071	0.201999
451.3886	0.017682	−0.006708	4.134220	0.329466
206.4890	0.054002	−0.020866	1.747603	0.361006
99.71711	0.133952	−0.053560	0.699543	0.271681
50.02856	0.255397	−0.106564	0.251587	0.104956
25.75606	0.344825	−0.152668		
13.49952	0.272048	−0.101290		
7.051286	0.094279	0.132675		
3.601607	0.010299	0.390156		
1.790316	0.001321	0.418524		
0.858850	0.000244	0.202308		
0.356872	0.000067	0.024676		

Table CXCVII. Zn ^1S $(23s15p11d)$ basis set. Energy(E_H) = −1777.848045

	s space			
Exponent	1s	2s	3s	4s
	−353.304500	−44.361690	−5.637790	−0.292495
29917080.	0.000001	0.000000	0.000000	0.000000
4476643.	0.000009	−0.000003	0.000001	0.000000
1017976.	0.000045	−0.000014	0.000005	−0.000001
288174.9	0.000192	−0.000059	0.000022	−0.000005
93987.85	0.000699	−0.000216	0.000082	−0.000016
33928.46	0.002282	−0.000706	0.000267	−0.000053
13234.12	0.006809	−0.002120	0.000802	−0.000161
5490.569	0.018734	−0.005887	0.002226	−0.000445
2396.228	0.047282	−0.015234	0.005788	−0.001162
1091.036	0.107135	−0.036167	0.013792	−0.002761
514.8647	0.207114	−0.077253	0.029905	−0.006022
250.5454	0.309817	−0.138804	0.054848	−0.011015
125.0976	0.297345	−0.184699	0.076775	−0.015643
63.41043	0.135560	−0.089556	0.039128	−0.007829
30.52619	0.016435	0.271780	−0.141181	0.029081
15.66241	−0.000272	0.558881	−0.414699	0.091628
8.032998	0.000349	0.313129	−0.297496	0.065318
3.772706	−0.000175	0.038708	0.355502	−0.091516
1.814118	0.000034	0.000538	0.674677	−0.218160
0.835025	−0.000021	0.000879	0.279393	−0.186082
0.196775	0.000005	−0.000088	0.008890	0.318962
0.085860	−0.000004	0.000067	−0.003354	0.586924
0.036698	0.000001	−0.000021	0.000879	0.249876

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−38.924810	−3.839349		−0.782513
35979.91	0.000021	−0.000008	639.7212	0.000208
8513.222	0.000184	−0.000069	192.6631	0.001954
2764.979	0.001073	−0.000402	74.84295	0.010711
1058.742	0.004829	−0.001814	32.86052	0.039058
450.2005	0.017759	−0.006738	15.39349	0.104848
205.9238	0.054224	−0.020953	7.525542	0.204568
99.43511	0.134418	−0.053758	3.715417	0.285213
49.88519	0.255965	−0.106820	1.806447	0.301444
25.68459	0.344892	−0.152746	0.852974	0.246226
13.46474	0.271295	−0.100642	0.384764	0.139026
7.035142	0.093689	0.133478	0.159335	0.036255
3.597376	0.010212	0.389706		
1.790527	0.001325	0.417841		
0.859809	0.000243	0.202502		
0.357497	0.000068	0.024813		

Table CXCVIII. Zn ^1S $(23s16p8d)$ basis set. Energy(E_H) = −1777.846928

	s space			
Exponent	1s	2s	3s	4s
	−353.304200	−44.361260	−5.637334	−0.292335
29563910.	0.000001	0.000000	0.000000	0.000000
4432605.	0.000009	−0.000003	0.000001	0.000000
1009744.	0.000046	−0.000014	0.000005	−0.000001
286234.7	0.000193	−0.000060	0.000023	−0.000005
93444.71	0.000703	−0.000218	0.000082	−0.000016
33755.16	0.002295	−0.000710	0.000268	−0.000054
13173.12	0.006845	−0.002131	0.000806	−0.000162
5467.418	0.018822	−0.005915	0.002237	−0.000447
2386.911	0.047477	−0.015300	0.005813	−0.001167
1087.097	0.107502	−0.036302	0.013844	−0.002771
513.1307	0.207616	−0.077488	0.029998	−0.006039
249.7557	0.310082	−0.139075	0.054964	−0.011036
124.7304	0.296822	−0.184678	0.076783	−0.015641
63.24221	0.134788	−0.088651	0.038743	−0.007748
30.45163	0.016257	0.273394	−0.142159	0.029280
15.62558	−0.000266	0.558831	−0.415248	0.091744
8.015726	0.000344	0.311699	−0.295932	0.064935
3.766632	−0.000174	0.038389	0.356948	−0.091860
1.811643	0.000033	0.000558	0.674022	−0.218058
0.834289	−0.000021	0.000871	0.278658	−0.185744
0.196908	0.000005	−0.000086	0.008867	0.317987
0.085958	−0.000004	0.000065	−0.003336	0.587249
0.036709	0.000001	−0.000021	0.000869	0.250517

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−38.924390	−3.838917		−0.782038
52867.93	0.000011	−0.000004	205.5981	0.002343
12511.79	0.000094	−0.000035	61.44593	0.018607
4065.286	0.000551	−0.000206	23.05643	0.077102
1557.595	0.002511	−0.000941	9.577756	0.202025
663.2892	0.009470	−0.003572	4.133609	0.329485
304.1561	0.030169	−0.011535	1.747324	0.361001
147.3680	0.080855	−0.031668	0.699427	0.271652
74.45469	0.175140	−0.071238	0.251547	0.104926
38.71493	0.289716	−0.123393		
20.57022	0.329850	−0.147396		
11.05425	0.209293	−0.044944		
5.874661	0.056259	0.206190		
3.052936	0.005053	0.408706		
1.547225	0.000996	0.374276		
0.754151	0.000185	0.154994		
0.306873	0.000045	0.015224		

Table CXCIX. Zn ^1S $(24s16p12d)$ basis set. Energy(E_H) = −1777.848087

	s space			
Exponent	1s	2s	3s	4s
	−353.304500	−44.361710	−5.637804	−0.292500
46857750.	0.000001	0.000000	0.000000	0.000000
7016731.	0.000005	−0.000002	0.000001	0.000000
1597149.	0.000026	−0.000008	0.000003	−0.000001
452509.0	0.000109	−0.000034	0.000013	−0.000002
147672.1	0.000397	−0.000123	0.000046	−0.000009
53330.17	0.001299	−0.000402	0.000152	−0.000030
20808.38	0.003891	−0.001207	0.000456	−0.000091
8634.929	0.010798	−0.003374	0.001276	−0.000256
3769.179	0.027808	−0.008815	0.003338	−0.000668
1716.525	0.065686	−0.021499	0.008180	−0.001643
810.2952	0.138117	−0.048096	0.018423	−0.003688
394.3235	0.243106	−0.095736	0.037288	−0.007519
196.9059	0.318477	−0.157049	0.062934	−0.012648
100.2442	0.250663	−0.174282	0.073728	−0.015098
51.40855	0.082664	−0.016517	0.007137	−0.001216
26.26431	0.005687	0.359201	−0.198936	0.041345
13.75761	0.000899	0.532705	−0.427798	0.095705
7.200903	−0.000280	0.240888	−0.211439	0.044848
3.500747	0.000090	0.025673	0.414217	−0.106302
1.709247	−0.000083	0.001294	0.643863	−0.216876
0.803012	0.000019	0.000541	0.247757	−0.172782
0.198488	−0.000007	−0.000013	0.007562	0.318499
0.085901	0.000005	0.000014	−0.002640	0.590498
0.036626	−0.000001	−0.000005	0.000684	0.248867

	p space		d space	
Exponent	2p	3p	Exponent	3d
	−38.924830	−3.839362		−0.782526
52392.39	0.000011	−0.000004	909.3783	0.000096
12395.86	0.000096	−0.000036	274.5726	0.000929
4026.308	0.000560	−0.000209	106.8660	0.005382
1542.201	0.002554	−0.000958	47.37161	0.021347
656.5443	0.009633	−0.003634	22.50319	0.062324
300.9678	0.030673	−0.011731	11.18995	0.139868
145.7740	0.082092	−0.032168	5.705634	0.230453
73.61894	0.177327	−0.072183	2.904547	0.284518
38.25783	0.292015	−0.124492	1.452580	0.277390
20.31317	0.329575	−0.147257	0.706452	0.211485
10.90358	0.205881	−0.040629	0.329043	0.110225
5.781507	0.053897	0.213205	0.141474	0.025659
3.001648	0.004683	0.410908		
1.522162	0.000980	0.369321		
0.742898	0.000174	0.149963		
0.301188	0.000044	0.014359		

Table CC. Ga ^2P $(20s15p9d)$ basis set. Energy(E_H) = −1923.260286

	s space			
Exponent	1s	2s	3s	4s
	−378.818200	−48.168190	−6.394429	−0.424476
6542455.	0.000008	−0.000002	0.000001	0.000000
979693.9	0.000062	−0.000019	0.000007	−0.000002
222951.0	0.000328	−0.000102	0.000039	−0.000009
63148.64	0.001383	−0.000429	0.000164	−0.000038
20600.49	0.005011	−0.001562	0.000596	−0.000139
7436.155	0.016097	−0.005059	0.001934	−0.000450
2899.506	0.046119	−0.014840	0.005682	−0.001322
1201.725	0.115500	−0.039050	0.015068	−0.003512
523.0896	0.237909	−0.089913	0.035113	−0.008190
236.8476	0.353567	−0.166768	0.067272	−0.015778
110.2491	0.291053	−0.200293	0.084986	−0.020021
51.15880	0.080509	0.013216	−0.005517	0.001188
24.36357	0.000628	0.497541	−0.303246	0.075485
11.73112	0.001635	0.528086	−0.481826	0.125587
5.318754	−0.000763	0.109762	0.093424	−0.031165
2.484193	0.000317	−0.000771	0.729866	−0.250042
1.093787	−0.000131	0.002207	0.425416	−0.283052
0.256212	0.000050	−0.000481	0.019810	0.332959
0.122585	−0.000037	0.000355	−0.008318	0.587482
0.052768	0.000011	−0.000105	0.002022	0.255904

	p space			d space	
Exponent	2p	3p	4p	Exponent	3d
	−42.493800	−4.482150	−0.208436		−1.193146
14674.34	0.000111	−0.000042	0.000007	363.1434	0.000876
3475.150	0.000985	−0.000374	0.000061	108.9187	0.007688
1128.375	0.005583	−0.002127	0.000347	41.83054	0.036437
430.9483	0.023664	−0.009134	0.001503	17.86490	0.113359
182.1980	0.078141	−0.030868	0.005046	8.114108	0.237820
82.61648	0.194884	−0.080409	0.013335	3.733427	0.333079
39.18813	0.341167	−0.148426	0.024428	1.681599	0.331216
19.18321	0.357275	−0.159887	0.027098	0.726153	0.218818
9.496871	0.164200	0.045694	−0.011950	0.284852	0.065126
4.548531	0.021822	0.388047	−0.073597		
2.115479	0.001384	0.481070	−0.105867		
0.944570	0.000335	0.217894	−0.036304		
0.301536	0.000029	0.015289	0.248902		
0.110556	−0.000008	−0.001816	0.550799		
0.039852	0.000002	0.000639	0.351816		

Table CCI. Ga ^2P ($21s16p11d$) basis set. Energy(E_H) = -1923.260738

	s space			
Exponent	1s	2s	3s	4s
	−378.818300	−48.168320	−6.394558	−0.424532
11280660.	0.000004	−0.000001	0.000001	0.000000
1689168.	0.000032	−0.000010	0.000004	−0.000001
384417.2	0.000166	−0.000051	0.000020	−0.000005
108888.0	0.000701	−0.000217	0.000083	−0.000019
35524.67	0.002548	−0.000793	0.000303	−0.000070
12825.11	0.008257	−0.002580	0.000984	−0.000229
5002.055	0.024172	−0.007658	0.002931	−0.000683
2074.448	0.063608	−0.020740	0.007951	−0.001849
904.3413	0.145693	−0.050747	0.019665	−0.004590
410.6592	0.270285	−0.107348	0.042165	−0.009831
192.6824	0.349210	−0.180646	0.073860	−0.017384
92.07610	0.237554	−0.173739	0.074780	−0.017581
42.05770	0.048122	0.110693	−0.053340	0.012508
21.07262	−0.002297	0.541834	−0.357364	0.090332
10.44881	0.001791	0.446892	−0.425141	0.110489
4.777393	−0.000828	0.076222	0.201113	−0.061215
2.282456	0.000355	−0.000944	0.714611	−0.256188
1.035248	−0.000141	0.001782	0.368773	−0.260360
0.257674	0.000050	−0.000348	0.015377	0.349331
0.119166	−0.000035	0.000242	−0.005734	0.595722
0.051285	0.000011	−0.000073	0.001426	0.236625

	p space			d space	
Exponent	2p	3p	4p	Exponent	3d
	−42.493930	−4.482274	−0.208467		−1.193275
22071.04	0.000055	−0.000021	0.000003	530.6813	0.000388
5225.112	0.000486	−0.000184	0.000030	159.5222	0.003570
1697.065	0.002796	−0.001063	0.000175	61.79780	0.018583
649.1857	0.012226	−0.004689	0.000763	26.86372	0.063777
275.2799	0.042709	−0.016633	0.002743	12.46225	0.157300
125.4136	0.118663	−0.047788	0.007810	5.980455	0.268197
60.07524	0.248580	−0.104526	0.017420	2.860390	0.325369
29.72822	0.360243	−0.161332	0.026491	1.336497	0.291513
15.03975	0.295072	−0.114334	0.019397	0.599223	0.172085
7.571398	0.098466	0.145968	−0.031324	0.244454	0.044142
3.738135	0.008759	0.427236	−0.080169		
1.796543	0.001397	0.423991	−0.100165		
0.829826	0.000077	0.159899	−0.010568		
0.272860	0.000069	0.009504	0.284319		
0.101539	−0.000030	−0.000861	0.545753		
0.037656	0.000009	0.000349	0.314055		

Table CCII. Ge ^3P $(20s15p9d)$ basis set. Energy(E_H) = −2075.359023

	s space			
Exponent	1s	2s	3s	4s
	−405.244200	−52.150130	−7.190791	−0.553251
7424671.	0.000007	−0.000002	0.000001	0.000000
1111788.	0.000058	−0.000018	0.000007	−0.000002
253011.8	0.000303	−0.000094	0.000036	−0.000009
71663.52	0.001279	−0.000398	0.000154	−0.000039
23378.57	0.004637	−0.001450	0.000559	−0.000143
8439.207	0.014914	−0.004697	0.001814	−0.000465
3290.842	0.042859	−0.013816	0.005347	−0.001371
1364.175	0.108109	−0.036471	0.014203	−0.003648
594.0974	0.225984	−0.084814	0.033458	−0.008601
269.3443	0.346414	−0.159862	0.064897	−0.016772
125.9235	0.303255	−0.203312	0.086964	−0.022584
59.59554	0.096921	−0.021200	0.010105	−0.002786
27.81032	0.003692	0.462193	−0.276354	0.075697
13.41519	0.001116	0.554354	−0.499211	0.143671
6.245327	−0.000525	0.136291	0.019548	−0.010489
2.882406	0.000199	0.001878	0.723694	−0.272684
1.278871	−0.000097	0.002112	0.474512	−0.337356
0.330838	0.000040	−0.000476	0.026568	0.314437
0.163049	−0.000028	0.000331	−0.009895	0.613149
0.069712	0.000008	−0.000094	0.002247	0.270901

	p space			d space	
Exponent	2p	3p	4p	Exponent	3d
	−46.235950	−5.161403	−0.287266		−1.634692
16283.96	0.000105	−0.000040	0.000008	420.7175	0.000783
3856.194	0.000925	−0.000357	0.000071	126.2834	0.006964
1252.157	0.005254	−0.002031	0.000399	48.63374	0.033742
478.3475	0.022357	−0.008758	0.001739	20.86967	0.107236
202.3414	0.074333	−0.029778	0.005872	9.537531	0.231675
91.83597	0.187598	−0.078484	0.015717	4.433559	0.333921
43.63820	0.334398	−0.147457	0.029289	2.027807	0.337151
21.41316	0.361110	−0.165074	0.033851	0.894575	0.216941
10.64409	0.175478	0.030203	−0.011361	0.357770	0.058844
5.124720	0.025610	0.376583	−0.087065		
2.408028	0.001399	0.487936	−0.132251		
1.096125	0.000390	0.227701	−0.046174		
0.373095	0.000005	0.017185	0.292722		
0.144802	0.000000	−0.001825	0.558326		
0.054457	−0.000002	0.000648	0.298864		

Table CCIII. Ge ^3P $(21s16p10d)$ basis set. Energy(E_H) = −2075.359458

	s space			
Exponent	1s	2s	3s	4s
	−405.244300	−52.150240	−7.190905	−0.553303
12425670.	0.000004	−0.000001	0.000001	0.000000
1860498.	0.000030	−0.000009	0.000004	−0.000001
423393.5	0.000159	−0.000050	0.000019	−0.000005
119926.6	0.000673	−0.000209	0.000081	−0.000021
39125.97	0.002447	−0.000763	0.000294	−0.000076
14125.29	0.007931	−0.002486	0.000958	−0.000245
5509.169	0.023242	−0.007382	0.002855	−0.000733
2284.762	0.061302	−0.020031	0.007761	−0.001989
996.0400	0.141131	−0.049147	0.019232	−0.004948
452.3130	0.264481	−0.104712	0.041554	−0.010676
212.2503	0.348674	−0.178346	0.073535	−0.019083
101.5324	0.246033	−0.179308	0.077975	−0.020202
46.91653	0.053708	0.087269	−0.042299	0.010821
23.50384	−0.001884	0.527440	−0.345024	0.096287
11.67616	0.001826	0.467783	−0.445578	0.127971
5.431760	−0.000859	0.089060	0.151716	−0.050784
2.607568	0.000373	−0.000339	0.717393	−0.285349
1.198048	−0.000156	0.001910	0.403220	−0.306389
0.329847	0.000059	−0.000408	0.019721	0.349074
0.155416	−0.000039	0.000261	−0.006311	0.616269
0.066900	0.000011	−0.000077	0.001519	0.241150

	p space			d space	
Exponent	2p	3p	4p	Exponent	3d
	−46.236070	−5.161511	−0.287306		−1.634806
23984.82	0.000053	−0.000020	0.000004	615.2990	0.000345
5677.834	0.000473	−0.000182	0.000036	185.1251	0.003207
1844.068	0.002724	−0.001051	0.000208	71.81612	0.017010
705.4626	0.011933	−0.004647	0.000914	31.34285	0.059594
299.2086	0.041799	−0.016524	0.003285	14.60574	0.150538
136.3674	0.116625	−0.047677	0.009417	7.059018	0.264490
65.37083	0.245835	−0.104971	0.021092	3.412662	0.328946
32.38853	0.359093	−0.163362	0.032497	1.619400	0.296619
16.41394	0.297755	−0.118072	0.023991	0.740284	0.168082
8.286942	0.101749	0.142069	−0.037130	0.306087	0.038844
4.112127	0.009401	0.427475	−0.098824		
1.998578	0.001435	0.425581	−0.123558		
0.944172	0.000035	0.158151	−0.010991		
0.341203	0.000077	0.009907	0.326854		
0.134350	−0.000035	−0.000538	0.546206		
0.051734	0.000010	0.000274	0.266728		

Table CCIV. As ^4S $(20s15p9d)$ basis set. Energy(E_H) = −2234.237946

	s space			
Exponent	1s	2s	3s	4s
	−432.586000	−56.309630	−8.029423	−0.685783
8462792.	0.000007	−0.000002	0.000001	0.000000
1267228.	0.000053	−0.000016	0.000006	−0.000002
288385.5	0.000278	−0.000087	0.000034	−0.000009
81683.31	0.001174	−0.000366	0.000143	−0.000039
26647.68	0.004257	−0.001335	0.000521	−0.000143
9619.619	0.013710	−0.004327	0.001687	−0.000465
3751.449	0.039519	−0.012756	0.004991	−0.001375
1555.462	0.100413	−0.033790	0.013281	−0.003664
677.8005	0.213082	−0.079347	0.031617	−0.008732
307.7340	0.337192	−0.152082	0.062125	−0.017239
144.4815	0.314821	−0.204299	0.088025	−0.024563
69.31261	0.116637	−0.053554	0.024787	−0.007105
31.63180	0.007684	0.421874	−0.247935	0.072795
15.32056	0.000391	0.574634	−0.509080	0.157568
7.298162	−0.000182	0.167312	−0.050620	0.012789
3.309903	0.000038	0.005753	0.710248	−0.286865
1.480152	−0.000041	0.001787	0.519708	−0.386770
0.416240	0.000017	−0.000376	0.034071	0.282410
0.208434	−0.000011	0.000240	−0.011058	0.644438
0.088182	0.000003	−0.000069	0.002392	0.289772

	p space			d space	
Exponent	2p	3p	4p	Exponent	3d
	−50.153550	−5.880507	−0.369384		−2.112460
17874.34	0.000100	−0.000039	0.000009	479.2546	0.000717
4232.673	0.000882	−0.000345	0.000077	143.9506	0.006442
1374.446	0.005016	−0.001969	0.000437	55.54968	0.031772
525.1676	0.021412	−0.008511	0.001907	23.92895	0.102749
222.2371	0.071566	−0.029083	0.006475	10.98863	0.227112
100.9394	0.182249	−0.077329	0.017483	5.148718	0.334825
48.03034	0.329283	−0.147293	0.033066	2.383253	0.341814
23.61351	0.363551	−0.169285	0.039207	1.068455	0.214597
11.77400	0.183792	0.019168	−0.010282	0.432805	0.054080
5.697191	0.028667	0.368843	−0.097519		
2.702715	0.001425	0.492891	−0.153229		
1.251952	0.000427	0.233104	−0.054030		
0.451201	−0.000014	0.018574	0.320593		
0.181066	0.000008	−0.001816	0.560461		
0.069765	−0.000004	0.000517	0.270299		

Table CCV. As ^4S $(21s16p10d)$ basis set. Energy(E_H) = −2234.238373

	s space			
Exponent	1s	2s	3s	4s
	−432.586100	−56.309740	−8.029536	−0.685838
13666450.	0.000004	−0.000001	0.000001	0.000000
2046160.	0.000029	−0.000009	0.000004	−0.000001
465630.8	0.000153	−0.000048	0.000019	−0.000005
131888.4	0.000646	−0.000202	0.000079	−0.000022
43028.13	0.002348	−0.000735	0.000286	−0.000079
15533.97	0.007614	−0.002394	0.000933	−0.000257
6058.566	0.022334	−0.007111	0.002778	−0.000766
2512.616	0.059039	−0.019330	0.007569	−0.002083
1095.405	0.136598	−0.047549	0.018791	−0.005195
497.4773	0.258512	−0.102006	0.040897	−0.011286
233.5028	0.347582	−0.175756	0.073084	−0.020381
111.8540	0.254319	−0.184237	0.080915	−0.022521
52.30259	0.059912	0.064383	−0.031397	0.008493
26.15255	−0.001240	0.511315	−0.331987	0.099643
13.01433	0.001808	0.487350	−0.463888	0.143470
6.151410	−0.000861	0.103187	0.104300	−0.037391
2.957543	0.000375	0.000623	0.718321	−0.308643
1.373345	−0.000166	0.001975	0.434920	−0.347663
0.408813	0.000065	−0.000450	0.024355	0.340807
0.194443	−0.000041	0.000263	−0.006656	0.638109
0.083616	0.000012	−0.000077	0.001588	0.248791

	p space			d space	
Exponent	2p	3p	4p	Exponent	3d
	−50.153660	−5.880611	−0.369433		−2.112572
25468.91	0.000054	−0.000021	0.000005	701.3744	0.000315
6029.112	0.000478	−0.000187	0.000041	211.1800	0.002947
1958.143	0.002751	−0.001077	0.000241	82.00665	0.015864
749.1131	0.012051	−0.004764	0.001059	35.89969	0.056540
317.7502	0.042223	−0.016949	0.003800	16.79007	0.145536
144.8457	0.117764	−0.048922	0.010927	8.159324	0.261785
69.45520	0.247874	−0.107609	0.024389	3.977442	0.332018
34.43170	0.360281	−0.166836	0.037624	1.910306	0.300352
17.45809	0.295413	−0.116835	0.026496	0.885876	0.164137
8.809618	0.099215	0.151363	−0.044525	0.369319	0.034975
4.379636	0.008797	0.437073	−0.116735		
2.145008	0.001446	0.419766	−0.140954		
1.029684	−0.000044	0.143872	−0.001294		
0.404727	0.000094	0.008618	0.361950		
0.165657	−0.000043	−0.000175	0.538945		
0.065618	0.000012	0.000068	0.233666		

Table CCVI. Se ^3P $(20s15p9d)$ basis set. Energy(E_H) = −2399.866873

	s space			
Exponent	1s	2s	3s	4s
	−460.867200	−60.668660	−8.931884	−0.837246
9549925.	0.000006	−0.000002	0.000001	0.000000
1429995.	0.000049	−0.000015	0.000006	−0.000002
325424.7	0.000258	−0.000081	0.000032	−0.000009
92174.51	0.001088	−0.000341	0.000134	−0.000039
30070.56	0.003947	−0.001242	0.000489	−0.000143
10855.55	0.012727	−0.004025	0.001585	−0.000464
4233.720	0.036781	−0.011889	0.004700	−0.001375
1755.742	0.094020	−0.031589	0.012532	−0.003670
765.4259	0.202042	−0.074763	0.030086	−0.008820
347.8811	0.328307	−0.145408	0.059812	−0.017615
163.7585	0.323630	−0.203892	0.088498	−0.026212
79.00418	0.134754	−0.078265	0.036126	−0.010930
35.47661	0.011597	0.385627	−0.224296	0.069848
17.27919	−0.000324	0.586264	−0.512399	0.168407
8.363609	0.000157	0.196518	−0.106908	0.034211
3.735947	−0.000114	0.009902	0.694389	−0.298603
1.686931	0.000019	0.001324	0.554873	−0.431578
0.506675	−0.000011	−0.000214	0.040755	0.268029
0.254078	0.000008	0.000114	−0.011471	0.673045
0.106276	−0.000002	−0.000039	0.002457	0.293614

	p space			d space	
Exponent	2p	3p	4p	Exponent	3d
	−54.268680	−6.661319	−0.402727		−2.649411
18850.79	0.000101	−0.000040	0.000010	539.6426	0.000667
4463.911	0.000898	−0.000356	0.000087	162.1869	0.006035
1449.526	0.005105	−0.002033	0.000489	62.68520	0.030217
553.8605	0.021791	−0.008787	0.002137	27.08932	0.099195
234.3982	0.072782	−0.030035	0.007260	12.48975	0.223448
106.4761	0.184938	−0.079696	0.019569	5.889985	0.335693
50.67590	0.332381	−0.151317	0.036916	2.753314	0.345671
24.92574	0.362190	−0.170482	0.042904	1.250496	0.212297
12.43064	0.178841	0.027524	−0.013977	0.511798	0.050140
6.035672	0.026985	0.380306	−0.110255		
2.886247	0.001424	0.490604	−0.171484		
1.359629	0.000341	0.217460	−0.043173		
0.517753	−0.000006	0.016840	0.356198		
0.206937	−0.000004	−0.000736	0.547550		
0.078752	−0.000003	0.000471	0.253471		

Table CCVII. Se ^3P $(21s16p10d)$ basis set. Energy(E_H) = −2399.867316

	s space			
Exponent	1s	2s	3s	4s
	−460.867300	−60.668790	−8.932021	−0.837329
15009610.	0.000004	−0.000001	0.000000	0.000000
2247283.	0.000028	−0.000009	0.000003	−0.000001
511410.2	0.000147	−0.000046	0.000018	−0.000005
144856.4	0.000619	−0.000194	0.000076	−0.000022
47258.68	0.002251	−0.000706	0.000278	−0.000081
17061.13	0.007303	−0.002303	0.000907	−0.000265
6654.157	0.021446	−0.006843	0.002700	−0.000791
2759.641	0.056814	−0.018634	0.007373	−0.002154
1203.156	0.132087	−0.045954	0.018337	−0.005381
546.4877	0.252376	−0.099233	0.040187	−0.011771
256.6067	0.345926	−0.172885	0.072488	−0.021463
123.1320	0.262365	−0.188488	0.083559	−0.024689
58.25891	0.066784	0.042303	−0.020782	0.005783
29.02094	−0.000336	0.493701	−0.318376	0.101530
14.46443	0.001728	0.505240	−0.479806	0.157844
6.934466	−0.000830	0.118410	0.059321	−0.022429
3.329714	0.000358	0.001950	0.717454	−0.329119
1.559881	−0.000167	0.001967	0.463807	−0.387304
0.492848	0.000068	−0.000465	0.028980	0.340241
0.235202	−0.000040	0.000247	−0.006799	0.658923
0.100350	0.000011	−0.000074	0.001642	0.249083

	p space			d space	
Exponent	2p	3p	4p	Exponent	3d
	−54.268810	−6.661443	−0.402807		−2.649546
25230.69	0.000061	−0.000024	0.000006	789.4310	0.000293
5973.089	0.000542	−0.000215	0.000052	237.8384	0.002752
1939.911	0.003115	−0.001237	0.000300	92.42965	0.014993
742.0169	0.013588	−0.005457	0.001319	40.56005	0.054223
314.6430	0.047247	−0.019280	0.004682	19.02659	0.141749
143.3760	0.129712	−0.054939	0.013366	9.286543	0.259882
68.68062	0.265649	−0.117752	0.028914	4.556957	0.334817
34.00918	0.367353	−0.174072	0.042943	2.210179	0.303098
17.19139	0.274907	−0.095699	0.022361	1.036672	0.160227
8.576914	0.079242	0.205819	−0.063562	0.434660	0.031649
4.221812	0.005144	0.473532	−0.143599		
2.052624	0.001332	0.383292	−0.144773		
0.961902	−0.000203	0.092157	0.062951		
0.421574	0.000128	0.002447	0.411707		
0.176275	−0.000061	0.001191	0.497323		
0.070665	0.000014	−0.000088	0.194735		

Table CCVIII. Br ^2P $(20s15p9d)$ basis set. Energy(E_H) = −2572.440569

	s space			
Exponent	1s	2s	3s	4s
	−490.060100	−65.199740	−9.871672	−0.992540
10636410.	0.000006	−0.000002	0.000001	0.000000
1592686.	0.000046	−0.000015	0.000006	−0.000002
362450.0	0.000242	−0.000076	0.000030	−0.000009
102662.5	0.001023	−0.000321	0.000128	−0.000039
33492.57	0.003712	−0.001171	0.000466	−0.000143
12091.20	0.011979	−0.003797	0.001510	−0.000463
4715.861	0.034688	−0.011229	0.004485	−0.001375
1955.920	0.089085	−0.029914	0.011978	−0.003677
852.9404	0.193342	−0.071226	0.028939	−0.008893
387.8817	0.320764	−0.140226	0.058118	−0.017943
182.8030	0.329956	−0.203032	0.088792	−0.027566
88.30908	0.149628	−0.096326	0.044620	−0.014131
39.28269	0.015044	0.355379	−0.205726	0.067167
19.24626	−0.000925	0.592170	−0.512561	0.176621
9.413770	0.000441	0.222006	−0.151547	0.053156
4.161912	−0.000241	0.013839	0.678597	−0.307495
1.900240	0.000074	0.000828	0.582183	−0.470100
0.604351	−0.000037	−0.000040	0.046914	0.255364
0.301469	0.000024	−0.000011	−0.011310	0.697547
0.125285	−0.000006	−0.000012	0.002467	0.297545

	p space			d space	
Exponent	2p	3p	4p	Exponent	3d
	−58.554000	−7.478002	−0.456950		−3.219957
19599.99	0.000105	−0.000042	0.000011	601.6184	0.000627
4641.388	0.000933	−0.000375	0.000097	180.9115	0.005717
1507.128	0.005304	−0.002142	0.000553	70.00902	0.028985
575.8389	0.022618	−0.009248	0.002407	30.33558	0.096392
243.6900	0.075338	−0.031567	0.008181	14.03339	0.220579
110.6842	0.190316	−0.083303	0.021899	6.653422	0.336597
52.66552	0.338139	−0.156767	0.041069	3.135910	0.348833
25.89695	0.359424	−0.170280	0.045775	1.439329	0.209878
12.89541	0.169634	0.043422	−0.019972	0.593426	0.046953
6.271607	0.023758	0.399715	−0.126123		
3.016111	0.001416	0.485261	−0.187237		
1.437646	0.000207	0.193128	−0.024273		
0.580404	0.000017	0.013983	0.386173		
0.234433	−0.000023	0.000387	0.535334		
0.089784	−0.000001	0.000416	0.233451		

Table CCIX. Br ^2P ($21s16p10d$) basis set. Energy(E_H) = −2572.441030

	s space			
Exponent	1s	2s	3s	4s
	−490.060200	−65.199880	−9.871817	−0.992631
16471300.	0.000003	−0.000001	0.000000	0.000000
2466255.	0.000027	−0.000008	0.000003	−0.000001
561243.7	0.000140	−0.000044	0.000018	−0.000005
158972.5	0.000593	−0.000186	0.000074	−0.000023
51864.88	0.002156	−0.000678	0.000270	−0.000083
18724.51	0.006997	−0.002213	0.000880	−0.000269
7303.119	0.020565	−0.006575	0.002620	−0.000804
3028.910	0.054596	−0.017935	0.007168	−0.002195
1320.672	0.127534	−0.044336	0.017858	−0.005494
599.9885	0.245986	−0.096353	0.039398	−0.012097
281.8774	0.343664	−0.169693	0.071715	−0.022264
135.5294	0.270229	−0.192068	0.085885	−0.026605
64.86140	0.074471	0.020919	−0.010411	0.002765
32.12644	0.000866	0.474528	−0.304041	0.101691
16.03607	0.001582	0.521460	−0.493303	0.170406
7.783901	−0.000764	0.134783	0.016168	−0.006248
3.724420	0.000323	0.003645	0.714684	−0.345285
1.758214	−0.000160	0.001889	0.490422	−0.423436
0.583177	0.000066	−0.000460	0.033754	0.335708
0.278483	−0.000038	0.000218	−0.006798	0.677883
0.118269	0.000010	−0.000068	0.001693	0.252159

	p space			d space	
Exponent	2p	3p	4p	Exponent	3d
	−58.554140	−7.478135	−0.457042		−3.220100
26596.19	0.000062	−0.000025	0.000006	879.9315	0.000275
6296.347	0.000550	−0.000221	0.000057	265.2498	0.002599
2044.884	0.003162	−0.001274	0.000330	103.1481	0.014299
782.1715	0.013795	−0.005617	0.001456	45.35262	0.052375
331.6889	0.047957	−0.019850	0.005156	21.32938	0.138727
151.1632	0.131490	−0.056517	0.014752	10.44892	0.258388
72.42474	0.268459	−0.120886	0.031753	5.156262	0.337251
35.88010	0.368311	−0.177288	0.047060	2.521753	0.305182
18.14296	0.271297	−0.092305	0.022437	1.193647	0.156659
9.047126	0.076321	0.218554	−0.071966	0.502250	0.029098
4.451674	0.004686	0.485491	−0.162626		
2.166659	0.001257	0.372356	−0.149745		
0.996600	−0.000235	0.077737	0.106413		
0.454421	0.000133	0.000670	0.436111		
0.194035	−0.000069	0.001795	0.467988		
0.079007	0.000014	−0.000065	0.169170		

Table CCX. Kr ^1S $(20s15p9d)$ basis set. Energy(E_H) = −2752.054193

	s space			
Exponent	1s	2s	3s	4s
	−520.165200	−69.902880	−10.849260	−1.152803
11707780.	0.000006	−0.000002	0.000001	0.000000
1753066.	0.000044	−0.000014	0.000005	−0.000002
398944.5	0.000231	−0.000073	0.000029	−0.000009
112999.2	0.000974	−0.000307	0.000123	−0.000039
36864.87	0.003535	−0.001118	0.000449	−0.000143
13308.71	0.011416	−0.003627	0.001456	−0.000464
5190.815	0.033109	−0.010736	0.004329	−0.001379
2153.030	0.085340	−0.028662	0.011581	−0.003695
939.0354	0.186645	−0.068559	0.028114	−0.008978
427.1455	0.314662	−0.136320	0.056948	−0.018275
201.3803	0.334441	−0.202145	0.089083	−0.028740
97.25352	0.161365	−0.109572	0.051069	−0.016807
43.05568	0.017976	0.330773	−0.191338	0.064979
21.20981	−0.001403	0.594870	−0.511732	0.183296
10.44568	0.000668	0.243453	−0.187221	0.069789
4.590763	−0.000344	0.017397	0.664307	−0.314904
2.120284	0.000124	0.000345	0.603560	−0.503613
0.708177	−0.000060	0.000121	0.052575	0.246066
0.350378	0.000037	−0.000122	−0.010782	0.717644
0.145189	−0.000009	0.000010	0.002449	0.300787

	p space			d space	
Exponent	2p	3p	4p	Exponent	3d
	−63.009570	−8.331304	−0.524059		−3.825027
20287.98	0.000110	−0.000045	0.000012	665.4865	0.000596
4804.425	0.000975	−0.000397	0.000108	200.2157	0.005457
1560.044	0.005536	−0.002267	0.000615	77.55788	0.027972
596.0170	0.023573	−0.009771	0.002669	33.68369	0.094094
252.2107	0.078266	−0.033293	0.009078	15.62728	0.218238
114.5310	0.196381	−0.087310	0.024098	7.443059	0.337470
54.47323	0.344370	−0.162590	0.044906	3.533089	0.351481
26.76773	0.355975	−0.169233	0.047554	1.635930	0.207515
13.29432	0.159614	0.062372	−0.027115	0.678227	0.044341
6.465053	0.020347	0.422526	−0.143152		
3.117679	0.001408	0.478436	−0.199052		
1.488649	0.000057	0.165770	0.003159		
0.635605	0.000060	0.009658	0.412841		
0.261244	−0.000030	0.000501	0.520387		
0.101608	0.000008	−0.000037	0.211890		

Table CCXI. Kr ^1S $(21s16p10d)$ basis set. Energy(E_H) = −2752.054669

	s space			
Exponent	1s	2s	3s	4s
	−520.165400	−69.903010	−10.849390	−1.152888
18075800.	0.000003	−0.000001	0.000000	0.000000
2705901.	0.000025	−0.000008	0.000003	−0.000001
615804.2	0.000134	−0.000042	0.000017	−0.000005
174431.8	0.000567	−0.000178	0.000072	−0.000023
56907.23	0.002062	−0.000650	0.000261	−0.000083
20544.04	0.006692	−0.002122	0.000852	−0.000271
8012.492	0.019690	−0.006308	0.002537	−0.000809
3323.085	0.052385	−0.017233	0.006954	−0.002213
1449.024	0.122950	−0.042704	0.017355	−0.005550
658.4398	0.239374	−0.093382	0.038535	−0.012297
309.5217	0.340820	−0.166225	0.070776	−0.022839
149.1392	0.277857	−0.194944	0.087862	−0.028293
72.11803	0.082970	0.000490	−0.000433	−0.000413
35.46657	0.002356	0.454030	−0.289161	0.100537
17.73073	0.001376	0.535748	−0.504259	0.181273
8.698467	−0.000666	0.152124	−0.025145	0.010584
4.140906	0.000273	0.005693	0.710009	−0.357881
1.968443	−0.000145	0.001740	0.515016	−0.456761
0.679992	0.000062	−0.000433	0.038671	0.328778
0.324541	−0.000033	0.000177	−0.006684	0.695006
0.137478	0.000009	−0.000061	0.001741	0.257000

	p space			d space	
Exponent	2p	3p	4p	Exponent	3d
	−63.009710	−8.331430	−0.524143		−3.825162
28660.16	0.000060	−0.000025	0.000007	973.1378	0.000261
6779.996	0.000537	−0.000219	0.000060	293.5010	0.002475
2201.021	0.003090	−0.001261	0.000343	114.2000	0.013729
841.7269	0.013504	−0.005571	0.001518	50.29608	0.050849
356.9445	0.047068	−0.019742	0.005385	23.70798	0.136225
162.7006	0.129571	−0.056426	0.015487	11.65147	0.257165
77.99035	0.266073	−0.121472	0.033512	5.777708	0.339416
38.67042	0.367836	−0.179503	0.050195	2.845995	0.306814
19.57986	0.274111	−0.096289	0.024472	1.357262	0.153423
9.792578	0.078738	0.216296	−0.075287	0.572458	0.027076
4.835471	0.004984	0.490013	−0.176070		
2.368015	0.001227	0.372690	−0.157071		
1.089829	−0.000245	0.074987	0.130527		
0.504512	0.000144	−0.000228	0.450239		
0.218430	−0.000062	0.001323	0.451281		
0.089952	0.000017	−0.000272	0.154217		

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16. Abstract

Energy-optimized, near Hartree-Fock quality gaussian type orbital (GTO) basis sets are reported for the first-row (Li to Ne) and third-row (K to Kr) atoms. The most accurate basis sets reported for the first row are (18*s* 13*p*) sets which are with 4 μE_H of the numerical Hartree-Fock (NHF) results. For B to Ne basis sets with more than 15*s* functions are quadruple zeta in the valence space. For the first-row transition metal atoms the (20*s* 12*p* 9*d*) basis sets are triple zeta in the valence space and are approximately equivalent to Clementi and Roetti's accurate Slater type orbital sets. Supplementing the (20*s* 12*p* 9*d*) basis sets optimized for the lowest state with the $4s^2 3d^n$ occupation with a diffuse *d* function gives self-consistent-field energy separations to the $4s^1 3d^{n+1}$ and $3d^{n+2}$ states which are within 100 μE_H of the NHF results. The most accurate basis sets for the transition metal atoms are with 30 μE_H of the NHF results. In addition, energy optimized sets are reported for He(^3P), Li(^2P) and Be(^3P).

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